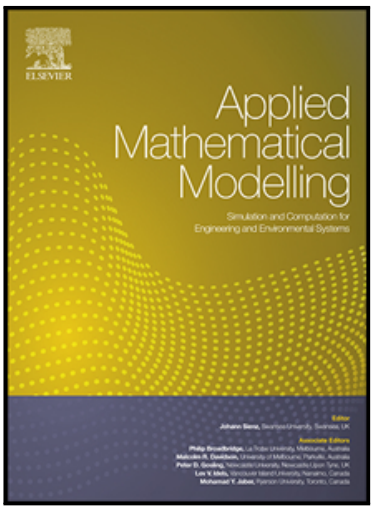
# Accepted Manuscript

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**Highlights**

- A rigorous analysis of high dimensional parameter sampling techniques
- New theoretical bounds for percentage coverage of parameter space by sampling
- Numerical simulations confirming bounds on percentage coverage of parameter space and applications of the coverage formula
- Results verifying t-way interactions coverage estimates in an experimental design setting depend on t not the total dimension

# Estimates of the coverage of parameter space by Latin Hypercube and Orthogonal Array-based sampling

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**Abstract**

In this paper we use counting arguments to prove that the expected percentage coverage of a $d$ dimensional parameter space of size $n$ when performing $k$ trials with either Latin Hypercube sampling or Orthogonal Array-based Latin Hypercube sampling is the same. We then extend these results to an experimental design setting by projecting onto a $t < d$ dimensional subspace. These results are confirmed by simulations. The theory presented has both theoretical and practical significance in modelling and simulation science when sampling over high dimensional spaces.

*Keywords:* Latin Hypercube sampling, Orthogonal Array-based Latin Hypercube sampling, Sample Space Coverage, Simulations

## 1. Introduction

Efficient and robust mechanisms for sampling high dimensional spaces are now a cornerstone of simulation and computational science, and arise

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in many different ways that we now briefly discuss. From a modelling and simulation perspective, increasing model complexity and computational demands together with a move towards quantifying the uncertainty in the data underpinning the model, has led to the development of surrogate models or emulators [1, 2]. The construction of these emulators requires the computationally intensive codes to be trained on an appropriate distribution of points in parameter space and then tested at a different set of points in order to capture the response surface appropriately [1]. In the case of uncertainty quantification, a quantity, either a random variable or a random response, is often expressed in some basis expansion (Hermite polynomials, for example) and the coefficients can be estimated using some sampling technique. Such an approach has been used, for instance, to forecast reservoir-performance in the petroleum industry [3] and to conduct a buckling analysis of a joined-wing model [4]. In many cases uncertainty can stem not only from deficiency of measured data, but also from physical properties such as the heterogeneity of geological formations or buckling response and aeroelastic complications under the effect of compressive loads.

In a different setting there may be a high level of uncertainty in the measured data and then the calibration of an ensemble or population of models over a high dimensional parameter space can provide deep insights into the underlying variability that underpins the model [5] - see more details later in this section. This approach is sometimes called a population of models (POM). In addition, a sensitivity analysis of parameter subsets is often important in ascertaining key parameters within the model [6]. Finally, Monte Carlo simulations for approximating high dimensional integrals is another area in which effective sampling is important.

The key aspect in all of these approaches is how to sample high dimensional spaces appropriately and effectively. Of course what is meant by these last two adverbs depends on the questions being asked. This leads us to the concept of experimental design for simulation experiments, [7, 8] and the criteria for assessing good or even optimal designs [9]. These criteria can include space filling, orthogonality (to assess impact of pairs of parameters) and noise reduction (to smooth the response surface). In the context of space-filling designs, criteria based on potential energy, the Euclidean maximum distance, discrepancy and D-optimality are commonly used - see [1] for a good discussion. In the context of orthogonality-based criteria, the essential idea is to minimise the correlation between variables. Most of these approaches depend on trying to find "so-called" optimal designs, which in themselves can

be highly computationally intensive and depend on the dimension of the underlying computational or parameter space and the sampling technique used [9, 7, 8].

In addressing this latter issue, we return to a brief discussion on the different types of sampling techniques. Perhaps the most popular technique is Latin Hypercube sampling (LHS). LHS was first introduced by McKay, Beckman and Conover [10]. Suppose that a $d$ dimensional parameter space is divided into $n$ equally sized subdivisions in each dimension then a Latin Hypercube trial (LHT) is a set of $n$ random samples with one from each subdivision; that is, each sample is the only one in each axis-aligned hyperplane containing it. A variant of LHS is known as Orthogonal Array-based Latin Hypercube sampling (OALHS) as introduced by Tang [11], and based on work in [12]. See also Leary et al. [13] for optimal constructions. This approach adds the requirement that for each trial the entire sample space must be sampled evenly at some coarse resolution.

An advantage of LHS is that it stratifies each univariate margin simultaneously, while Stein [14] showed that with LHS there is a form of variance reduction compared with uniform random sampling. Tang [11] suggested that it may also be important to stratify the bivariate margins. For instance, an Experimental Design may involve a large number of variables, but in reality only a relatively small number of these variables are effective. One way of dealing with this problem has been to project the factors onto a subspace spanned by the effective variables. However this can result in a replication of sample points within the effective subspace. Welch et al. [15] suggested LHS as a method for screening for effective factors, but there is still no guarantee, even in the case of bivariate margins, that this projection is uniformly distributed. On the other hand, OALHS achieves uniformity on small dimensional margins [11].

Additional sampling techniques are based on Sobol sequences and Hammersley sequences. These latter approaches give a low-discrepancy experimental design and provide a better uniform distribution than LHS. More recently, it has been pointed out that most sampling approaches generate the entire set of sample points in one attempt and this does not allow for flexibility or adaptivity. In [16] the authors introduce an approach called Progressive LHS in which a series of finer and finer, usually by doubling the sample size, LHSs are generated. This approach is a generalisation of Sliced LHS [17] in which a LHS is generated from a collection of smaller equally-sized LHSs.

We now return to the application that motivated our work, namely the building of a population of models. In the setting of a population of models (POM) a mathematical model is calibrated by a set of points, rather than a single point, in parameter space, all of which are selected to fit sets of experimental/observational data. The POM approach was originally proposed for neuroscience modelling [18], but has been recently extended to a variety of issues in cardiac electrophysiology. These include studies of inter-subject variability in cardiac cells [5], inter-subject variability in a population of rabbit ventricular action potentials [19], inter-subject variability in human atrial action potential models [20], and mRNA expression levels in failing and non-failing human hearts [21]. In these settings, biomarker values are extracted and then the models are calibrated against these biomarkers. This calibration is usually against the ranges of the biomarkers but, more recently, calibration was done against the distribution of data values for each biomarker [22].

The POM approach leads to methodologies that are essentially probabilistic in nature and gives greater weight to the experimental, modelling, simulation feedback paradigm [23]. By implementing experiments based on a POM, as distinct from experiments based on a single model, the variability in the underlying structure can be captured by allowing changes in the parameter values. This avoids complications arising from decisions on the use of "best" or "mean" data, and the difficulties of identifying such data. We note that POM have similarities with Approximate Bayesian Computation (ABC) [24]. However, in ABC the sampling is usually performed adaptively so as to converge to subregions of parameter space where the calibrated models lie, as distinct from random sampling of the entire space.

Given this discussion it is clearly important to be able to estimate the expected coverage of parameter space using sampling techniques such as LHS or OALHS. Furthermore, it is also important to understand the relationship between Experimental Design and POM in this regard. For example, it may be desirable to know if a POM calibrates for interactions of "small strength" by checking for all possible combinations of levels for, say, pairs or triples of variables. This would equate to investigating the coverage of 2 and 3 dimensional subspaces.

In these settings the authors [25] focused on estimating the expected coverage of a 2 dimensional parameter space for a population of $k$ trials forming a LHS with each trial of size $n$. In particular, an incomplete counting argument was used to predict the expected coverage of points in the parameter space after $k$ trials of size $n$. These estimates were compared against numer-

ical results based on a MATLAB implementation of 100 simulations. The results of the simulations led the authors to conjecture that the expected percentage coverage by $k$ trials of a 2 dimensional parameter space tended to $1 - e^{-k/n}$.

In a later paper [26] the authors extended this work and reported on the expected coverage of $d$ dimensional space based on MATLAB implementations of simulations of LHS and OALHS. They also tested for uniform coverage of lower dimensional subspaces of dimension $t$. Let the expected coverage of parameter space be defined as

$$P(k, n, d, t) = \frac{U(k, n, d, t)}{n^d}, \tag{1}$$

where $U(k, n, d, t)$ is the expected number of cells in a parameter space of dimension $d$ with a partition size of $n$ with $k$ trials, projected onto a $t$ dimensional subspace. Then [26] conjectured that the expected coverage of a $t$ dimensional subspace of a $d$ dimensional parameter space of size $n$ when performing $k$ trials of LHS is $P(k, n, d, t) = 1-(1-1/n^{t-1})^k$ or $1-e^{-k/n^{t-1}}$ when $k$ is large, suggesting that the coverage is independent of $d$ when considering projections onto a subspace of smaller dimension $t$.

The aim of this present paper is to synthesise the results in [25, 26] to prove the above conjecture, to provide additional simulations demonstrating the result and to discuss how this estimate can be used in a practical setting. Thus in Section 2 we give some background on LHS and OALHS. Then in Section 3 we give formal counting arguments and prove that the conjectures given above are true. We provide counting arguments and use combinatorial techniques to find the expected coverage of parameter space when taking the union of $k$ trials in the case of LHS and OALHS. We extend these arguments in a natural manner to sub-block coverage when projecting onto a 2 dimensional subspace (Experimental Design). We also give theoretical bounds on the percentage coverage of parameter space for both LHS and OALHS (showing that they are equivalent with respect to the coverage). We then extend these estimates to the coverage when projecting down onto a 2 dimensional subspace. In Section 4 we present some simulation results that support our theoretical results and discuss how our results can be used in a practical setting. Finally, in Section 5 we give some concluding remarks.

## 2. Methods

We begin by reviewing the well known methods used to generate LHSs and formalise the definitions for OALHS. A LHT on $d$ variables each taking $n$ values from the set $[n] = \{1, 2, \ldots, n\}$ may be represented as an $n$ by $d$ matrix where each column is an arbitrary permutation of $[n]$, and with each row forming a $d$-tuple of the LHT. Thus a *Latin Hypercube trial* (LHT or a LH $d$-trial) is a randomly generated subset of $n$ points from a $d$ dimensional parameter space satisfying the condition that the projections onto each of the 1 dimensional subspaces are permutations. A collection of $k$ LH $d$-trials forms a *Latin Hypercube sample* (LHS).

LHT1

$$\begin{bmatrix} 1 & 2 & 1 \\ 2 & 3 & 3 \\ 3 & 1 & 2 \\ 4 & 7 & 8 \\ 5 & 8 & 5 \\ 6 & 5 & 4 \\ 7 & 4 & 6 \\ 8 & 6 & 7 \end{bmatrix}$$

LHT2

$$\begin{bmatrix} 1 & 3 & 2 \\ 2 & 4 & 6 \\ 3 & 5 & 3 \\ 4 & 7 & 8 \\ 5 & 1 & 1 \\ 6 & 2 & 7 \\ 7 & 8 & 4 \\ 8 & 6 & 5 \end{bmatrix}$$

LHT3

$$\begin{bmatrix} (1,1) & (1,2) & (1,1) \\ (1,2) & (1,3) & (1,3) \\ (1,3) & (1,1) & (1,2) \\ (1,4) & (2,3) & (2,4) \\ (2,1) & (2,4) & (2,1) \\ (2,2) & (2,1) & (1,4) \\ (2,3) & (1,4) & (2,2) \\ (2,4) & (2,2) & (2,3) \end{bmatrix}$$

OALHT4

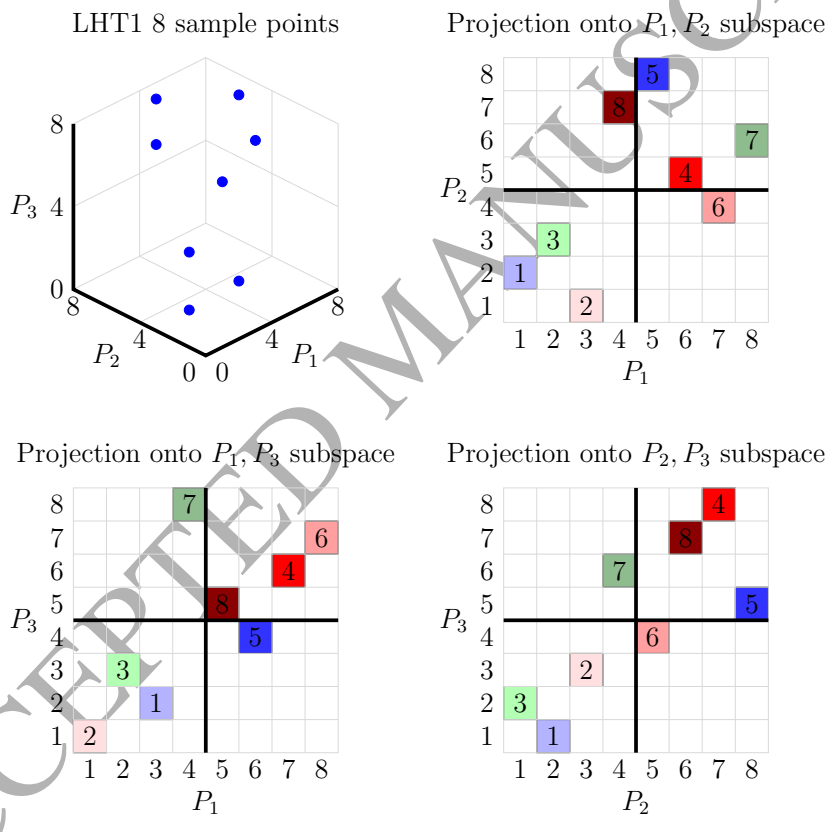
$$\begin{bmatrix} (1,1) & (1,3) & (1,2) \\ (1,2) & (1,4) & (2,2) \\ (1,3) & (2,1) & (1,3) \\ (1,4) & (2,3) & (2,4) \\ (2,1) & (1,1) & (1,1) \\ (2,2) & (1,2) & (2,3) \\ (2,3) & (2,4) & (1,4) \\ (2,4) & (2,2) & (2,1) \end{bmatrix}$$

By way of an example, the two matrices given above are two LH 3-trials on the set $\{1, 2, \ldots, 8\}$, denoted LHT1 and LHT2. Note that since a LH $d$-trial is a multiset it is invariant under any permutation of the rows. LH 3-trials, LHT1 and LHT2, may also be represented diagrammatically as illustrated in Fig. 1 and Fig. 2, respectively. Collectively the union of LHT1 and

LHT2 forms a LHS of $k = 2$ trials. Here the value of the third variable is represented by the colour:

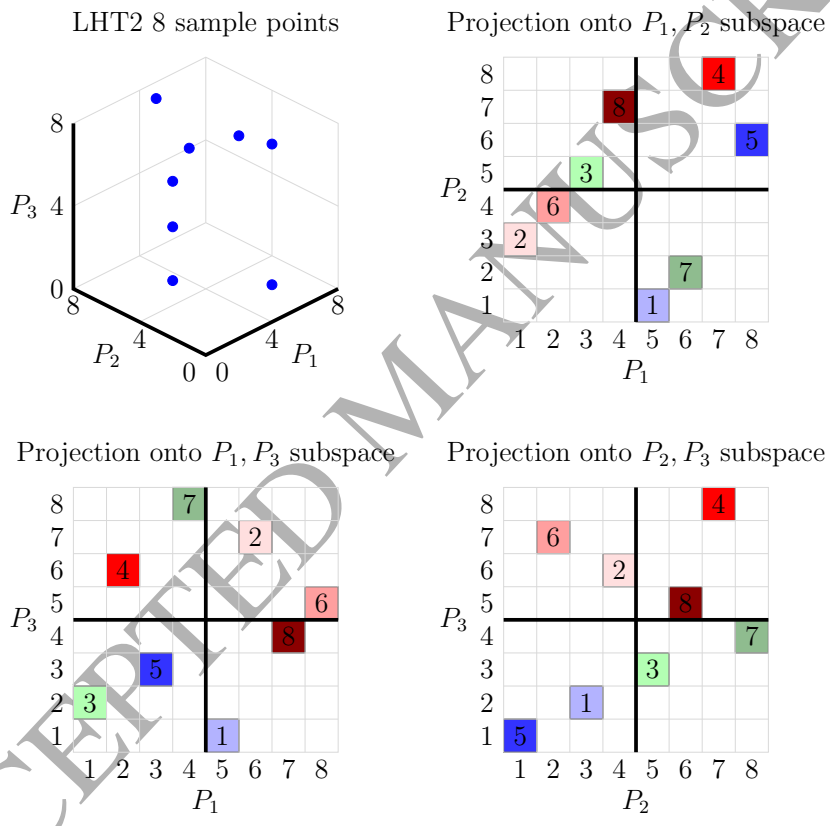
| Third Coordinate | | | | | | | |
|---|---|---|---|---|---|---|---|
| Light Blue | 1 | Light Pink | 2 | Light Green | 3 | Light Red | 4 |
| Dark Blue | 5 | Dark Pink | 6 | Dark Green | 7 | Dark Red | 8 |

Figure 1: Projections onto the 2 dimensional subspaces for LHT1.




While LHT1 and LHT2 are both examples of LH 3-trials they exhibit different properties. The 2 dimensional subspace defined by each of the pairs of variables $P_1$ and $P_2$, variables $P_1$ and $P_3$ and variables $P_2$ and $P_3$ can be partitioned into four equally sized sub-blocks as shown by the thicker lines

Figure 2: Projections onto the 2 dimensional subspaces for LHT2.



in Fig. 1 and Fig. 2. In LHT2 we see that the 3-tuples (points) are evenly distributed across the four sub-blocks, while this is not the case in LHT1.

The 3-trial LHT2 is an example of a specific space filling design known as an OALH $d$-trial, where the sample points achieve uniformity on the bivariate margins. With this example in mind it is useful to have a formal definition for sub-blocks, OALH $d$-trials and OALHS.

Let $n = p^d$ for some $p \in \mathbb{N}$. A $d$ dimensional parameter space (the set of all $n^d = p^{d^2}$ $d$-tuples), where each variable takes $n = p^d$ values, may be partitioned into $p^d$ *sub-blocks* each of which contain $p^{d^2}/p^d = p^{d(d-1)}$ points ($d$-tuples); that is, for each $(p_1, p_2, p_3, \ldots, p_d) \in [p]^d$, the set of $p^{d(d-1)}$ ordered $d$-tuples

$$SB_{(p_1,\ldots,p_d)} = \{((p_1, x_1), (p_2, x_2), \ldots, (p_d, x_d)) \mid x_i \in [p^{d-1}]\}$$

defines a *sub-block*. Note that $(p_i, x_i)$ is interpreted as $(p_i - 1)p^{d-1} + x_i$ and, in our examples, $p = 2$.

A LH $d$-trial is said to be an OALH $d$-trial if the $n$ $d$-tuples are distributed evenly across all sub-blocks. Formally, a LH $d$-trial $H$ is said to be an *Orthogonal Array-based Latin Hypercube $d$-trial* (OALH $d$-trial) if $n = p^d$ and for each of the $p^d$ $d$-tuples of the form $(p_1, p_2, \ldots, p_d)$, where $1 \leq p_i \leq p$, there exists an element of $H$ of the form $((p_1, x_1), (p_2, x_2), \ldots, (p_d, x_d))$, where $1 \leq x_i \leq p^{d-1}$ and $(p_i, x_i)$ is interpreted as $(p_i - 1)p^{d-1} + x_i$. Thus an OALH $d$-trial on $n = p^d$ values may be represented as an $n$ by $d$ matrix where each entry is an ordered pair $(x, y) \in [p] \times [p^{d-1}]$. Furthermore, when the matrix entries are restricted to the first coordinates, all $p^d$ $d$-tuples on the set $[p]$ are covered and when the rows of matrix are partitioned according to the first coordinate, for each partition, the second coordinate forms an arbitrary permutation of $[p^{d-1}]$ (that is, we have $p$ arbitrary permutations on the set $[p^{d-1}]$).

In the above example the entries of LHT1 and LHT2 have been rewritten as ordered pairs in LHT3 and LHT4, respectively, and it is easy to see that LHT4 (LHT2) is an OALH 3-trial, while LHT3 (LHT1) is not.

## 3. Theoretical Results

In this section we give theoretical arguments that calculate the expected coverage of the parameter space when taking the union of $k$ $d$-trials. To achieve this we begin by using combinatorial techniques to count the expected intersection sizes for a multiset of $m$ LH $d$-trials. These arguments

are presented below and then extended to the expected coverage based on OALH $d$-trials.

*3.1. The expected intersection size of LH d-trials*

As each coordinate in a LH $d$-trial contains each element of $[n]$ exactly once and a LH $d$-trial is invariant under row permutations, the number of LH $d$-trials on $[n]$ is $n!^{d-1}$.

Let $\mathcal{M}$ be the set of all selections of $m$ LH $d$-trials (with repetition retained in each of the selections, so $\mathcal{M}$ is a set of multisets each of size $m$). The number of ways to choose $q$ elements from a set of size $p$, with repetition, is $\binom{p+q-1}{q} = \binom{p+q-1}{p-1}$, so

$$|\mathcal{M}| = \binom{n!^{d-1} + m - 1}{m}. \tag{2}$$

**Theorem 3.1.** *Let $M$ be a multiset of $m$ LH $d$-trials on $[n]$; that is $M \in \mathcal{M}$. The expected number of ordered $d$-tuples common to all $m$ LH $d$-trials in $M$ is given by*

$$x_m(n) = n^d \binom{(n-1)!^{d-1} + m - 1}{m} \Big/ \binom{n!^{d-1} + m - 1}{m}. \tag{3}$$

*Proof.* Fix a $d$-tuple $\mathbf{a} = (a_1, a_2, \ldots, a_d) \in [n]^d$. There are $(n-1)!^{d-1}$ $d$-trials that contain this $d$-tuple. From this set the number of ways to choose, with repetition, $m$ of these $d$-trials is

$$t_{\mathbf{a}} = \binom{(n-1)!^{d-1} + m - 1}{m}.$$

That is, there are $t_{\mathbf{a}}$ choices of $m$ LH $d$-trials that have $\mathbf{a}$ in their intersection. For $M \in \mathcal{M}$ denote the number of $d$-tuples common to all LH $d$-trials in $M$ by $c(M)$. Then

$$\sum_{M \in \mathcal{M}} c(M) = \sum_{\mathbf{a} \in [n]^d} t_{\mathbf{a}} = n^d \binom{(n-1)!^{d-1} + m - 1}{m}.$$

Hence the expected number of ordered $d$-tuples common to all $m$ LH $d$-trials for an arbitrary $M \in \mathcal{M}$ is

$$\left( \sum_{M \in \mathcal{M}} c(M) \right) \frac{1}{|\mathcal{M}|} = n^d \binom{(n-1)!^{d-1} + m - 1}{m} \Big/ \binom{n!^{(d-1)} + m - 1}{m}.$$

□

*3.2. The expected intersection size of OALH d-trials*

For general $d$ we count the number of OALH $d$-trials. Thus the assumption is that $n = p^d$. Let $H$ be an OALH $d$-trial. Recall that for each $d$-tuple $(p_1, p_2, , \ldots, p_d) \in [p]^d$ there is precisely one element of $H$ of the form

$$((p_1, x_1), (p_2, x_2), \ldots, (p_d, x_d)),$$

where $x_i \in [p^{d-1}]$. All elements of $H$ are of this form for some $(p_1, p_2, , \ldots, p_d)$ in $[p]^d$.

It will be useful to talk about individual coordinates in $H$ so for each $i = 1, \ldots, d$, let

$$H_i(j) = \{h \in H \mid \text{ the } i\text{-th coordinate of } h \text{ is } (j, x_i) \text{ for some } x_i \in [p^{d-1}]\}.$$

Since $H$ is a LH $d$-trial, $|H| = p^d = n = p \cdot p^{d-1}$ and for each $i = 1, \ldots, d$ and each $j = 1, \ldots, p$, $|H_i(j)| = n/p = p^{d-1}$.

**Lemma 3.2.** *The number of OALH d-trials on* $[p] \times [p^{d-1}]$ *is* $(p^{d-1})!^{dp}$.

*Proof.* Let $H$ be an OALH $d$-trial. There are $n = p^d$ $d$-tuples in $H$. Fix $i$ and $j$, where $1 \leq i \leq d$ and $1 \leq j \leq p$, and define a function $f_{ij} : [p^{d-1}] \to H_i(j)$, by

$$f_{ij}(y) = ((p_1, x_1), (p_2, x_2), \ldots, (j, y), \ldots, (p_d, x_d)),$$

where $(j, y)$ is the $i$-th coordinate. Since $f_{ij}$ is a one-to-one and onto function there are $(p^{d-1})!$ different functions to choose from and $dp$ choices for $i, j$ so $(p^{d-1})!^{pd}$ possible $d$-trials. □

**Lemma 3.3.** *A fixed d-tuple, say* $((p_1, x_1), (p_2, x_2), \ldots, (p_d, x_d))$, *occurs in*

$$p^{d(d-1)(p-1)}(p^{d-1} - 1)!^{dp}$$

*OALH d-trials on* $[p] \times [p^{d-1}]$.

*Proof.* By Lemma 3.2 there are $(p^{d-1})!^{pd}$ OALH $d$-trials, and each contains $n = p^d$ $d$-tuples. There are $n^d$ distinct $d$-tuples and any two occur the same number of times in the disjoint union of the $d$-trials. Hence a fixed $d$-tuple occurs in

$$\frac{(p^{d-1})!^{dp} \times n}{n^d} = (p^{d-1})!^{dp}/p^{d(d-1)} = p^{d(d-1)(p-1)}(p^{d-1} - 1)!^{dp}$$

OALH $d$-trials. □

Let $\mathcal{M}_o$ be the set of all selections of $m$ OALH $d$-trials (so $\mathcal{M}_o$ is a set of multisets each of size $m$). So by Lemma 3.2

$$|\mathcal{M}_o| = \binom{(p^{d-1})!^{dp} + m - 1}{m} = \binom{(n/p)!^{dp} + m - 1}{m}.$$

**Theorem 3.4.** *Let $M$ be a multiset of $m$ OALH $d$-trials on $[p] \times [p^{d-1}]$ where $n = p^d$; that is $M \in \mathcal{M}_o$. The expected number of ordered $d$-tuples common to all $m$ OALH $d$-trials is*

$$x_m(n) = p^{d^2} \binom{p^{d(d-1)(p-1)}(p^{d-1}-1)!^{dp} + m - 1}{m} \Big/ \binom{(p^{d-1})!^{dp} + m - 1}{m}.$$

*Proof.* The proof follows as in the proof of Theorem 3.1, except that we consider $\mathcal{M}_o$ instead of $\mathcal{M}$ and the number of OALH $d$-trials that intersect in a fixed $d$-tuple as established in Lemma 3.3.

□

*3.3. The expected size of edgewise intersection of LH d-trials*

Let $1 \leq i < j \leq d$. An $(i, j)$-*edge* of a $d$-tuple $\mathbf{a} = (a_1, a_2, \ldots, a_d)$ is an ordered pair $(a_i, a_j)$. Two LH $d$-trials, $H_1$ and $H_2$, are said to intersect in an $(i, j)$-edge $(a_i, a_j)$, if there exists $(a_1, a_2, \ldots, a_d) \in H_1$ and $(a'_1, a'_2, \ldots, a'_d) \in H_2$, such that $a_i = a'_i$ and $a_j = a'_j$.

There are $\binom{d}{2}$ edges in a $d$-tuple, so the total number of possible distinct edges is $n^2\binom{d}{2}$. In addition, there are $n$ $d$-tuples in a LH $d$-trial, so there are $n\binom{d}{2}$ edges in total in a $d$-trial.

**Lemma 3.5.** *A fixed $(i, j)$-edge $(a_i, a_j)$ is contained in $(n-1)!n!^{d-2}$ distinct LH $d$-trials.*

*Proof.* Multiplying the number of distinct LH $d$-trials by the number of edges in a LH $d$-trial and dividing by the total number of distinct edges counts the number of LH $d$-trials that contain a fixed $(i, j)$-edge; that is,

$$\frac{n!^{d-1} \times n\binom{d}{2}}{n^2\binom{d}{2}} = (n-1)!n!^{d-2}.$$

□

We now count the expected number of edges common to all LH $d$-trials from a selection $M \in \mathcal{M}$.

**Theorem 3.6.** *Let $M$ represent a multiset of $m$ LH $d$-trials on $[n]$; that is, $M \in \mathcal{M}$. Then the expected number of edges common to all $m$ LH $d$-trials in $M$ is*

$$x_m(n) = n^t \binom{d}{t} \binom{(n-1)!^{d-1} n^{d-2} + m - 1}{m} \Big/ \binom{n!^{d-1} + m - 1}{m}, \quad t = 2\,; \tag{4}$$

*that is, $x_m(n)$ is the expected intersection in the projection to a subspace of dimension $t = 2$.*

*Proof.* The case $d = 2$ is covered in Theorem 3.1. For general $d$ we fix an $(i, j)$-edge, say $(a_i, a_j)$. By Lemma 3.5 there are $(n-1)!n!^{d-2}$ LH $d$-trials that contain this edge. From this set the number of ways to choose, with repetition, $m$ of these LH $d$-trials is

$$s_{(a_i,a_j)} = \binom{(n-1)!(n!)^{d-2} + m - 1}{m}.$$

That is, there are $s_{(a_i,a_j)}$ choices of $m$ LH $d$-trials that intersect in the fixed $(i, j)$-edge $(a_i, a_j)$.

For $M \in \mathcal{M}$ denote the number of edges common to all LH $d$-trials by $c(M)$. Then, denoting the set of $(i, j)$-edges by $E$,

$$\sum_{M \in \mathcal{M}} c(M) = \sum_{1 \le i < j \le d} \left( \sum_{(a_i,a_j) \in E} s_{(a_i,a_j)} \right) = n^2 \binom{d}{2} \binom{(n-1)!(n!)^{d-2} + m - 1}{m}.$$

Hence the expected number of edges common to all $m$ LH $d$-trials for an arbitrary $M \in \mathcal{M}$ is

$$\left( \sum_{M \in \mathcal{M}} c(M) \right) \frac{1}{|\mathcal{M}|} = n^2 \binom{d}{2} \binom{(n-1)!n!^{d-2} + m - 1}{m} \Big/ \binom{(n!)^{d-1} + m - 1}{m}.$$

The result follows by noting that $(n-1)!n!^{d-2} = (n-1)!^{d-1} n^{d-2}$. □

In [26] the authors used MATLAB simulations to test the percentage coverage of $t$ dimensional subspaces at the sub-block level, where we recall

that for a $d$ dimensional parameter space with $n = p^d$, the set of $p^{d(d-1)}$ ordered $d$-tuples

$$SB_{(p_1,\ldots,p_d)} = \{((p_1, x_1), (p_2, x_2), \ldots, (p_d, x_d)) \mid x_i \in [p^{d-1}]\}$$

defines a sub-block. These simulations were focused on testing the percentage coverage for $(i, j)$-edges from the set

$$E_{(p_i,p_j)} = \{((p_i, x_i), (p_j, x_j)) \mid x_i, x_j \in [p^{d-1}]\},$$

where $i, j \in [d]$ and $p_i, p_j \in [p]$ are fixed. Note $|E_{(p_i,p_j)}| = (p^{d-1})^2$. Theorem 3.6 allows us to calculate the expected coverage of this set of $(i, j)$-edges.

**Corollary 3.7.** *Let $n = p^d$. Further let $M$ be a multiset of $m$ LH $d$-trials on $[p^d]$; that is $M \in \mathcal{M}$. Fix $i, j \in [d]$ and $p_i, p_j \in [p]$. Then the expected number of $(i, j)$-edges in $E_{(p_i,p_j)}$ and common to all $m$ LH $d$-trials in $M$ is*

$$x_m(n) = p^{2d-2}\binom{(p^d - 1)!^{d-1}p^{d^2-2d} + m - 1}{m} \Big/ \binom{p^d!^{d-1} + m - 1}{m}. \quad (5)$$

*Proof.* Theorem 3.6 gives the expected number of edges common to all $m$ LH $d$-trials in $M$ (that is, $i$ and $j$ are not fixed). However we are interested in the expected number of edges in $E_{(p_i,p_j)}$ (with $i$ and $j$ fixed). There are $\binom{d}{2}$ choices for the pair $(i, j)$, where $1 \le i < j \le d$. Also rather than summing over all $n^2 = p^{2d}$ $(i, j)$-edges we sum over the $p^{2d-2}$ edges in $E_{(p_i,p_j)}$. Therefore to evaluate $x_m(n)$ we divide the result from Theorem 3.6 by $p^2\binom{d}{2}$. □

**Remark:** There is a natural extension of this result to projection onto a subspace of arbitrary dimension $t > 2$.

### *3.4. Bounds on percentage coverage of d-tuples*

To estimate the number of cells in the parameter space covered by the union of $k$ $d$-trials, with $n$ partitions for each of the $d$ parameters, we count via the Principle of Inclusion/Exclusion obtaining

$$U(k, n, d, d) = \sum_{m=1}^{k} (-1)^{m+1} \binom{k}{m} x_m(n), \quad (6)$$

where $x_m(n)$ denotes the expected intersection size of $m$ arbitrary trials depending on the sampling strategy. We recall the definition of the expected

percentage coverage of parameter space given in (1). When there is no projection on to the $t$-dimensional subspace, we write

$$P(k,n,d,d) = \frac{U(k,n,d,d)}{n^d}. \tag{7}$$

We have from Theorems 3.1, 3.4 and 3.6 three different expressions for the $x_m(n)$. So let the expected numbers of ordered $d$-tuples in the case of LHS, OALHS and sub-block coverage for $t = 2$ be, respectively, $x_{mL}(n)$, $x_{mO}(n)$ and $x_{m2}(n)$ then from Theorems 3.1, 3.4 and 3.6 we have

$$\begin{aligned}
x_{mL}(n) &= n^d \prod_{i=0}^{m-1} \frac{a+i}{b+i}, \quad a = (n-1)!^{d-1}, \quad b = n!^{d-1} \\
x_{mO}(n) &= n^d \prod_{i=0}^{m-1} \frac{a+i}{b+i}, \quad a = p^{d(d-1)(p-1)}(p^{d-1}-1)!^{dp}, \quad b = (p^{d-1})!^{dp}; \text{ and} \\
x_{m2}(n) &= n^2 \prod_{i=0}^{m-1} \frac{a+i}{b+i}, \quad a = (n-1)!^{d-1}n^{d-2}, \quad b = n!^{d-1}.
\end{aligned}$$

Note that in the case that $d = 2$ then $x_{mL}(n) = x_{m2}(n)$.

Now the binomial expansion gives

$$\sum_{m=0}^{k} \binom{k}{m} u^m = (1+u)^k. \tag{8}$$

Also it is easy to see that, for $x \geq 0$,

$$1 + x \leq e^x \quad \text{and } 1 - e^{-x} \leq x, \tag{9}$$

while, for $0 \leq t < 1$,

$$e^{\frac{t}{2}} - 1 \leq t \quad \text{and } -\tfrac{t^2}{2} \leq t + \ln(1-t) \leq \tfrac{-t^2}{4}. \tag{10}$$

Moreover, for $0 < a \leq b$ and $i \geq 0$,

$$\frac{a}{b} \leq \frac{a+i}{b+i} \leq \frac{a}{b}\left(1 + \frac{i}{a}\right) \leq \frac{a}{b}\exp\left(\frac{i}{a}\right). \tag{11}$$

Thus for $0 \le i \le m-1 \le k-1$

$$\left(\frac{a}{b}\right)^m \le \prod_{i=0}^{m-1}\left(\frac{a+i}{b+i}\right) \le \left(\frac{a}{b}\right)^m \prod_{i=0}^{m-1}\left(1+\frac{i}{a}\right) \le \left(\frac{a}{b}\right)^m \exp\left(\frac{k(k-1)}{2a}\right), \quad (12)$$

and for $0 \le t = \frac{k(k-1)}{a} \le 1$, using (10)

$$0 \le \prod_{i=0}^{m-1}\left(\frac{a+i}{b+i}\right) - \left(\frac{a}{b}\right)^m \le \left(\frac{a}{b}\right)^m \left(\exp\left(\frac{k(k-1)}{2a}\right) - 1\right) \le \left(\frac{a}{b}\right)^m \frac{k(k-1)}{a}. \quad (13)$$

We relate this back to the expression for the $x_m(n)$ for a general $a$ and $b$ with $0 < a \le b$ and

$$x_m(n) = n^d \prod_{i=0}^{m-1} \frac{a+i}{b+i}.$$

Recalling that $P(k,n,d,d)$ denotes the expected coverage fraction of $d$-tuples in the parameter space by taking the union of $k$ $d$-trials with either LHS or OALHS, we have the following result.

**Theorem 3.8.** *In the case of LHS and OALHS (with $n = p^d$)*

$$P(k,n,d,d) \sim (1-\exp(-k\lambda)) \ \text{ as } k\lambda^2 \to 0, \quad \lambda = \frac{1}{n^{d-1}}. \quad (14)$$

*Proof.* We begin by using the Principle of Inclusion/Exclusion, using (8) and evaluating $P(k,n,d,d)$ in terms of the general form of $x_m(n)$, as follows

$$\begin{aligned} P(k,n,d,d) &= \sum_{m=1}^{k} (-1)^{m+1} \binom{k}{m} x_m(n)/n^d = \sum_{m=1}^{k} (-1)^{m+1} \binom{k}{m} \prod_{i=0}^{m-1} \frac{a+i}{b+i} \\ &= 1 - \sum_{m=0}^{k} (-1)^m \binom{k}{m} \lambda^m + E_1 = 1 - \exp(-k\lambda) + E_2 + E_1, \end{aligned}$$

where $\lambda = \frac{a}{b}$,

$$E_1 = \textstyle\sum_{m=1}^{k} (-1)^m \binom{k}{m} \left[\lambda^m - \prod_{i=0}^{m-1} \left(\frac{a+i}{b+i}\right)\right]$$

and

$$E_2 = \exp(-k\lambda) - (1-\lambda)^k.$$

It follows from (13) and then (8) and (9) that

$$|E_1| \leq \sum_{m=0}^{k} \binom{k}{m} \lambda^m \tfrac{k(k-1)}{a} \leq \exp(k\lambda) \tfrac{k(k-1)}{a}.$$

Moreover, it follows from (9) and (10) that

$$|E_2| = \exp(-k\lambda) \left|1 - \exp(k\lambda + k \ln(1-\lambda))\right| \leq \exp(-k\lambda) k\lambda^2.$$

As $n \to \infty$

$$\begin{aligned} E = E_1 + E_2 &= \mathrm{O}\left(1 - \exp(-k\lambda)\right) \text{ and} \\ E = E_1 + E_2 &= \mathrm{O}\left(\exp(-k\lambda)\right), \end{aligned}$$

provided $k\lambda \leq Cn$; note it follows from Stirling's formula that $\frac{e^{2k\lambda}k^2}{a} \to 0$ in this case. Thus

$$P(k, n, d, d) \sim \left(1 - \exp(-k\lambda)\right), \text{ as } k\lambda^2 \to 0.$$

Finally, in the case of LHS with $a = (n-1)!^{d-1}$ and $b = n!^{d-1}$ then

$$\lambda = \frac{1}{n^{d-1}};$$

while with OALHS $a = (p^{d-1}-1)!^{dp} p^{d(d-1)(p-1)}$ and $b = (p^{d-1})!^{dp}$ and so

$$\lambda = p^{d(d-1)(p-1)} \left(\tfrac{(p^{d-1}-1)!}{(p^{d-1})!}\right)^{dp} = p^{d(d-1)(p-1)-(d-1)dp} = \tfrac{1}{p^{d(d-1)}} = \tfrac{1}{n^{d-1}}.$$

Thus $\lambda$ is the same in both cases and the percentage coverage is the same in both cases (assuming that $n = p^d$ for the OALHS case) and so the result is proved. □

We can extend this analysis to the case of the 2 dimensional sub-block projection ($t = 2$) but now $P(k, n, d, 2) = \frac{U(k,n,d,2)}{n^2}$.

**Theorem 3.9.** *For the 2 dimensional sub-block projection*

$$P(k, n, d, 2) \sim \left(1 - \exp(-k\lambda)\right) \text{ as } k\lambda^2 \to 0, \quad \lambda = \frac{1}{n}. \tag{15}$$

*Proof.* With $a = (n-1)!^{d-1} n^{d-2}$ and $b = n!^{d-1}$ then

$$\lambda = \tfrac{(n-1)!^{d-1} n^{d-2}}{n!^{d-1}} = n^{d-2} \tfrac{(n-1)!^{d-1}}{n!^{d-1}} = \tfrac{1}{n}.$$

□

## 4. Simulation Results and Discussion

We now present some simulation results confirming our theoretical results. We had already given some simulation results in [26] where we first made our conjecture on the relationship between coverage, trials, and dimension. There we considered the case $d = 5$ and gave expected coverage at the 25, 50, 75 and 100 percent levels for $t = 2, 3, 4$ by plotting the logarithm of the number of trials as a function of the logarithm of $n$. We saw the expected linear relationship. We now give additional simulations for the case $d = 5$, $t = 4$ and $d = 6$, $t = 2, 3$, for the same expected percentage coverage - see Fig. 3.

Theorem 3.8 states that the expected coverage of both LHS and OALHS is of the form $1 - exp(-k\lambda)$ where $\lambda = \frac{1}{n^{d-1}}$, while Theorem 3.9 states that the expected coverage when projecting onto a $t$ dimensional subspace with $t = 2$ has the same form but now $\lambda = \frac{1}{n}$ and this coverage is independent of $d$. Although, we have not presented the analysis here we can extend the results of Theorem 3.9 to arbitrary $t$ so that $\lambda = \frac{1}{n^{t-1}}$. Fig.3 confirms these results. In all but the full coverage case the gradient of the straight line is $t - 1$. In the case of the full coverage the gradient appears to behave as $t - 1/2$. We think this is partly due to the effect that as the percentage coverage increases then the higher is the rate of overlapping $d$-trials. Nevertheless our numerical results are consistent with the theory.

We now give some brief comments on how our methodology can be used in practical settings. First we note that if TOL represents a designated percentage covering of the parameter space then we need to choose $k$ (the number of trials) and $n$ (the discretisation of parameter space) such that

$$1 - e^{-k/n^{d-1}} = \text{TOL}$$

or, after simplification

$$k = -n^{d-1} \ln(1 - \text{TOL}).$$

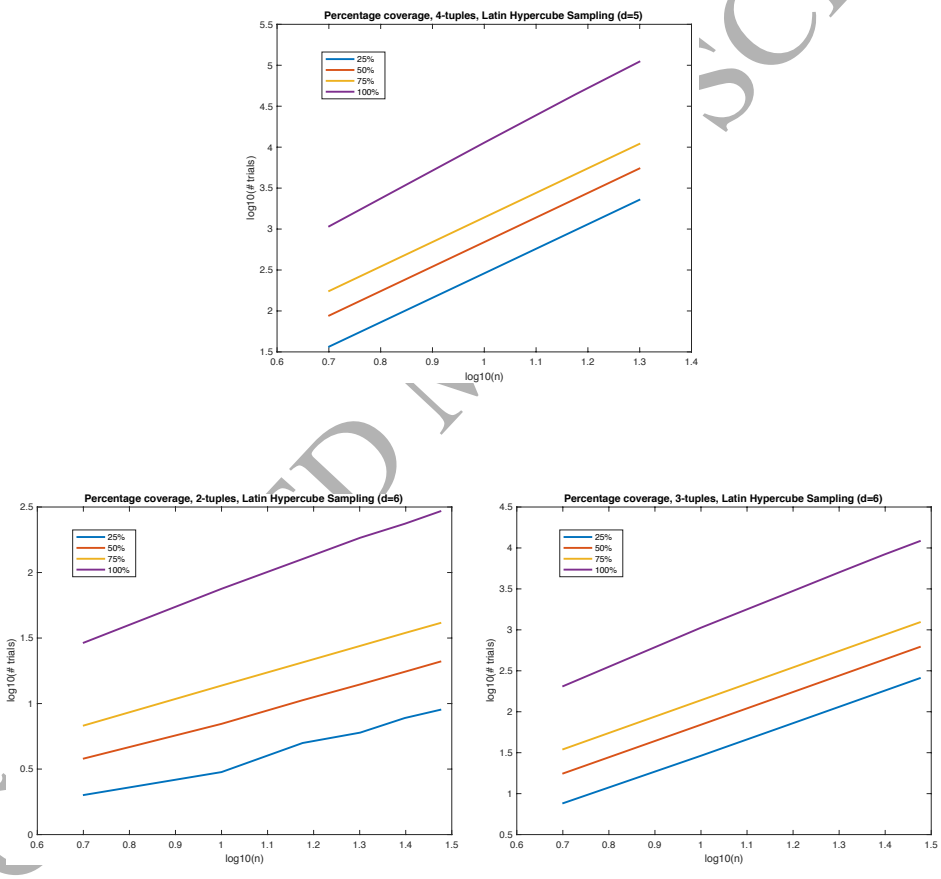
Assuming TOL is small, this gives

$$k \approx \text{TOL}\, n^{d-1}, \tag{16}$$

or with projection onto a $t$-dimensional subspace

$$k \approx \text{TOL}\, n^{t-1}. \tag{17}$$

Figure 3: Plots of the logarithm of the number of trials versus the logarithm of the discretisation of the parameter space for a $d = 5$-dimensional parameter space projected onto a $t = 4$-dimensional subspace and for a $d = 6$-dimensional parameter space projected onto $t = 2$ and 3 dimensional subspaces



In a very recent paper by some of these authors [22], our aim was to build a population of atrial electrophysiological models such that the outputs from this population matched as accurately as possible the actual distribution of values over 7 biomarkers on a cohort of 450 people. The number of parameters was 11. The 7 biomarkers correspond to different measurements associated with the propagation of an action potential wave. As a consequence, there are unknown correlations between some of the parameters so that the whole population of models lies on an unknown subspace of the full space. Some cursory inspection suggests that there are three-way correlations between three of the ion channel conductance parameters. In order to guarantee good coverage onto the projected $t = 3$ dimensional subspace, we choose a coverage of 25%. In addition, we had chosen $n = 50$ in order to build a suitably-sized population of models. Equation (17) then leads to

$$k \approx \frac{1}{4} 50^2$$

so that with a value for the number of trials of 625 we are able to analyse those possible three-way correlations thoroughly. This preliminary study allows us to improve the process of building a population of models on a high dimensional space (in this case, dimension 11) by effectively reducing the dimension of the full space due to these particular correlations.

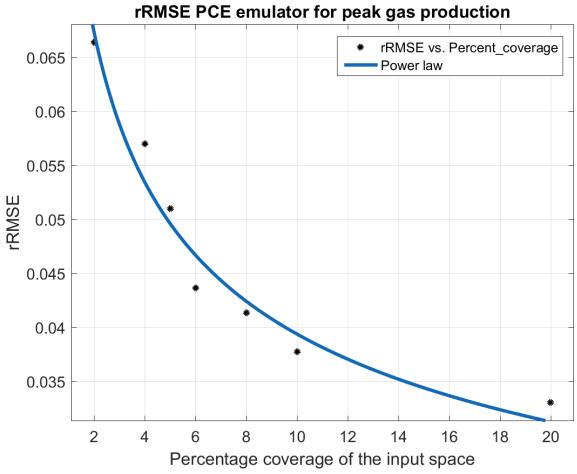
In a second application, where $n = 10$ and $d = 4$, estimate (16) was used to explore the relationship between coverage of a parameter space and the accuracy of an emulator used to forecast coal seam gas production. An emulator, based on an ordinary least squares implementation of a fifth order Polynomial Chaos Expansion (PCE), was built using a black box approach (data in and data out) to a standard industry software package [27], used for the prediction of gas production. The emulator accounted for uncertainty in four variables ($d = 4$) permeability, porosity, Langmuir volume and Langmuir pressure. Seven emulator response surfaces were built from input/output pairs obtained by running the original model at a set of training points, which were selected using LHS. The domain for each variable was divided into $n = 10$ subdivisions and seven emulators were built, with points coverage set at 2%, 4%, 5%, 6%, 8%, 10% and 20% of the input space. In each case the corresponding number of LHSs was calculated using estimate (16) and the relative root mean square error (rRMSE) was calculated by comparing the original model, $\mathcal{M}$, and the emulator, $\mathcal{P}$, at a further 65 LHS, approximately

6% of the input space, where

$$\text{rRMSE} = \sqrt{\frac{1}{n}\sum_{\mathbf{x}\in\mathcal{X}}\left(\frac{\mathcal{P}(\mathbf{x})-\mathcal{M}(\mathbf{x})}{\mathcal{M}(\mathbf{x})}\right)^2}. \tag{18}$$

The results are displayed in Fig. 4. These data suggest that the trend for rRMSE (as a function of percentage coverage) follows a power law rRMSE $= 0.08486x^{-0.3338}$. Such a power law expansion and estimate (16) could be used to investigate the relationship between the order of the PCE, the percentage coverage and the accuracy of the emulator. Without doing this, it is a rather hit-and-miss approach in order to get an idea of suitable coverage of parameter space in relation to the emulator accuracy.

Figure 4: Plots of the error convergence of a surrogate model when the number of training points are increased as a percentage of the parameter space.




In a different setting we could use estimate (16) as part of the iterative refinement approach, called Progressive LHS, described in [16]. Estimate (16) could be used to determine how many iterations and trials are needed in order to attain a given coverage at a given resolution of parameter space. This would make these approaches truly adaptive.

## 5. Conclusions

In conclusion, we have obtained analytical results for the expected coverage of parameter space when using both LHS and OALHS. We have shown that there is no difference between the two in terms of the expected coverage. We have also obtained analytical results of the expected coverage when projecting onto small dimension subspaces. In this case the expected coverage is independent of the dimension of the parameter space and depends only on the dimension of the projected subspace. The analytical results are also supported by simulations.

In addition, we have discussed several practical settings in which our results on the relationship between the number of trials, dimension and percentage coverage of space can be used. Of course one limitation of this study pertains to the curse of dimensionality. As the dimension $d$ of the parameter space increases, then clearly the percentage coverage as given in Theorem 3.8 becomes small; this may limit the practical use of the result in very large dimensions. However, this is not a fault of the theory. Nevertheless, even in this case Theorem 3.8 and Theorem 3.9 are powerful as they show that the expected coverage when projected into a smaller $t$ dimensional subspace follows the theory in that $d$ is replaced by $t$. In light of this, the results are very significant in practical situations, as the two scenario investigations in section 4 show.

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