U.S. ARMY COMBAT CAPABILITIES DEVELOPMENT COMMAND – ARMAMENTS CENTER

Screening Designs for Resource-Constrained Deterministic M&S Experiments: *An Ammunition Case Study*

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ACKNOWLEDGEMENTS

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OUTLINE

- **Background**
- **Objective**
- **Motivation**
  - Unique Problem
  - Historical Solutions
  - Proposed Solution
- **DACE Alternatives**
- **D-Optimal Latin Hypercube Designs (D-LHD)**
  - Joseph, Krishna, Ray, 2019
- **Case Study**
  - Test Design
  - Analysis
- **Conclusions & Future Work**

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BACKGROUND

- An Integrated Product Team (IPT) at the Combat Capabilities Development Command Armaments Center (CCDC AC) are developing a new small-caliber ammunition round

- Some of the details of this project are classified

- The team discovered some issues with the accuracy performance of the round during early prototype testing

- In an attempt to better describe the behavior and focus the team's engineering efforts on the most impactful factors and high technical risk areas, modeling and simulation was the best option available to investigate potential improvements

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BACKGROUND (CONT.)

- The model to assess these aeroballistics characteristics and resulting dispersion performance is highly complex, and takes substantial time to run on the HPCC
- The teams' overall goal was to screen the 19 factors of interest to determine which were the most important with regard to the resulting dispersion performance
- Only time for 25 simulations of the model, which includes a 'centerpoint' (baseline nominal condition across entire design space)

OBJECTIVE

- **Using deterministic computational modeling, the IPT expected to identify the significant factors with respect to dispersion performance**

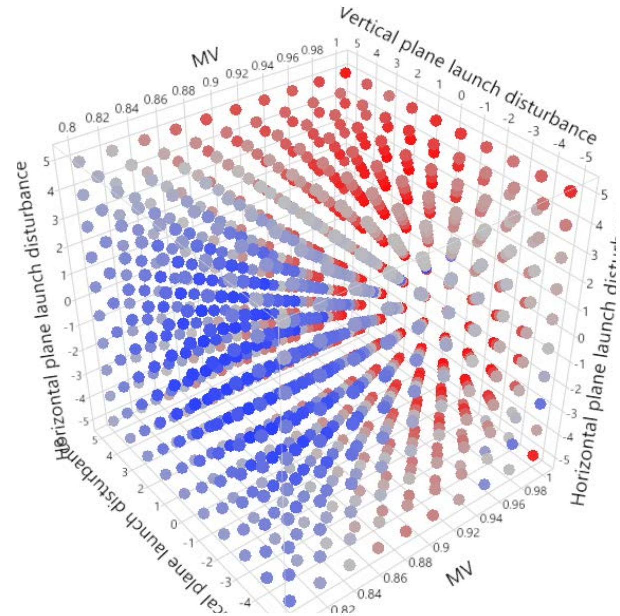
- **With these insights, the team would be able to focus their design engineering efforts on the highest impact variables in the hopes of making a substantial improvement to dispersion performance**

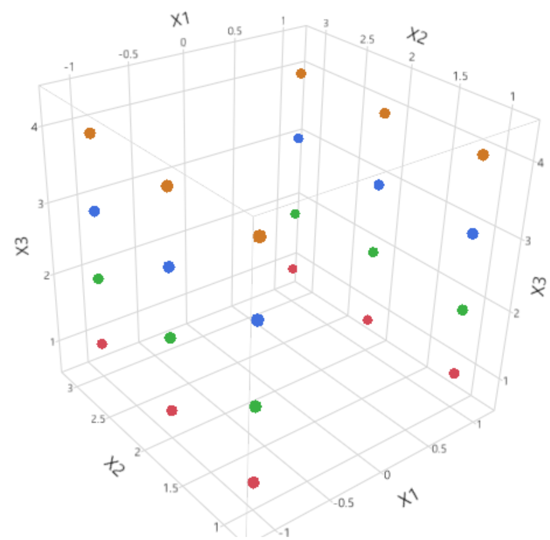
- **Simulating a model systematically at various input conditions throughout the design space provides a number of advantages:**
  – Model verification (both code and solution verification)
  – Generate a computationally inexpensive 'emulator'
  – Sensitivity analysis & tradespace exploration & optimization
  – Validate the model with live test data

- **Systematically simulating deterministic model using DOE is best-practice (Sacks et. al. 1989)**

COMMONLY ENCOUNTERED APPROACHES

- **Design space ‘grid’**
  - Dense-grid: 5+ levels
  - Sparse-grid: 2-4 levels (full-factorial)
  - These are often employed with fast-running models
  - Intuitive, simple, but inefficient and infeasible with more than a few factors due to sample size
  - Often no analysis, looking for largest or smallest number, or fitting trendlines
- **Also, OFAT and Direct Monte-Carlo (but the intent isn’t function approximation or optimization)**

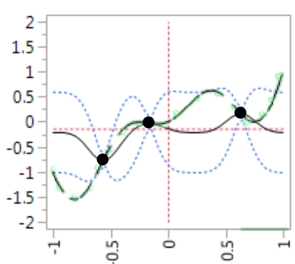




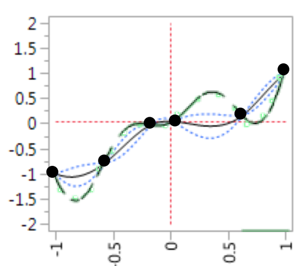
DOE FOR DETERMINISTIC M&S

- **Statistical approach to approximating underlying computational model involved sampling from the design space and then fusing statistical or machine-learning model to this data to generate an ‘emulator’ or surrogate for the underlying physics-based model**

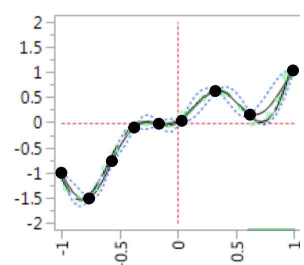
- **Space-Filling Designs have seen some advancement over the past few decades**
  - Intent is to uniformly fill the multidimensional space and all projections
  - Goal is to capture underlying model behavior, nonlinearities, and sensitivities
  - DOE approach informed by anticipated statistical modeling approach, usually intent is to use GASP/Kriging for model approximation in deterministic setting but regression can be a valid alternative, though some caveats and loss of efficiency (Jones, Johnson, 2009)



3 runs



6 runs



9 runs

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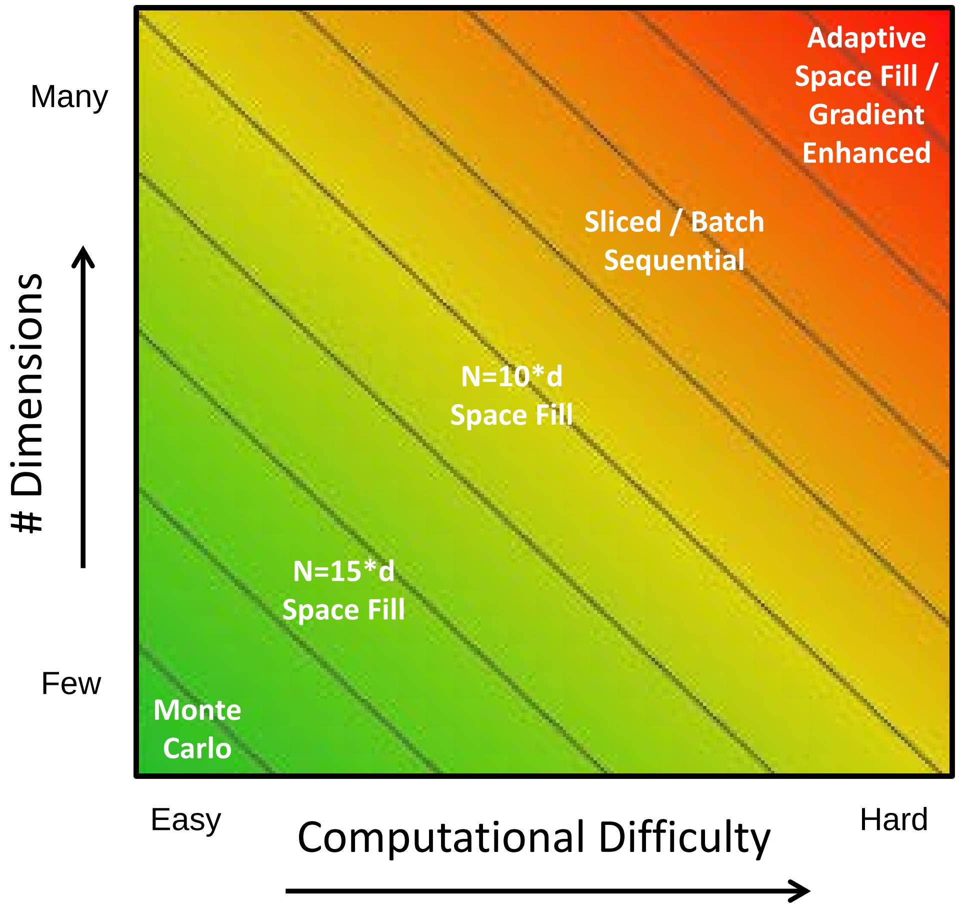
M&S DOE APPROACH



UQ M&S Objectives:

Screening/Ranking Effects
Characterization
Sensitivity Analysis & Variation Decomposition
Augment Test Data
Augmented with limited test data
Robust Optimization
Robust Optimization & Data Assimilation

Notes:

(1) This is oversimplified – there is no simple answer, the DOE approach must be tailored to the unique constraints of the M&S problem

(2) Though Space-Filling Designs (and therefore Kriging models) are emphasized here; there are certain situations where Factorial-based designs, and optimal designs (or combinations of Space-filling augmented by optimal design points) may be more appropriate, and Regression modeling techniques can be advantageous

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SPACE-FILLING DESIGNS

- **A simple design can be constructed using uniform Monte-Carlo simulation**
  – Possible to have gaps and clusters of data, especially in projection
- **Latin Hypercube Design is the workhorse**
  – Still some issues, no guarantees regarding design-space coverage, but ensures one-dimensional projections and n-dimensional stratification
- **miniMax design seeks to minimize the max distance point (Johnson, Moore and Ylvisaker, 1990)**
  – Combine miniMax LHD to enforce 1D projections
- **Maximin (sphere-packing) design spreads the points as far apart as possible in the space**
  – Easy to construct, combine Maximin LHD to enforce 1D projections, points pushed to boundaries of design space

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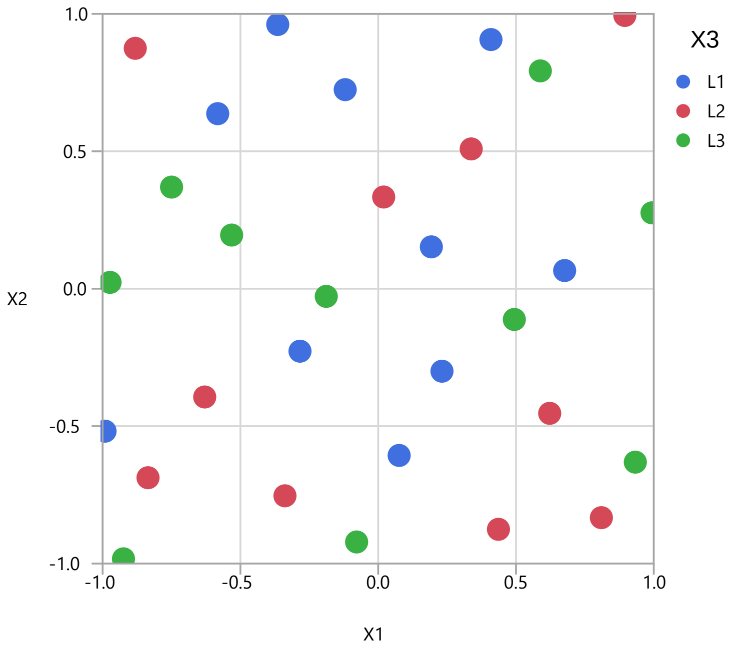
MAXPRO

- **MaxPro and MaxPro LHD's seek to optimally space the points in lower-dimensional projections (Joseph, Gul, Ba, 2015)**
  - MaxPro provide good projection and pushes points toward boundaries, MaxPro LHD provides more uniformity throughout the space

- **More recent extensions include MaxPro for categoric and ordinal factors (Joseph, Gul, Ba, 2018)**

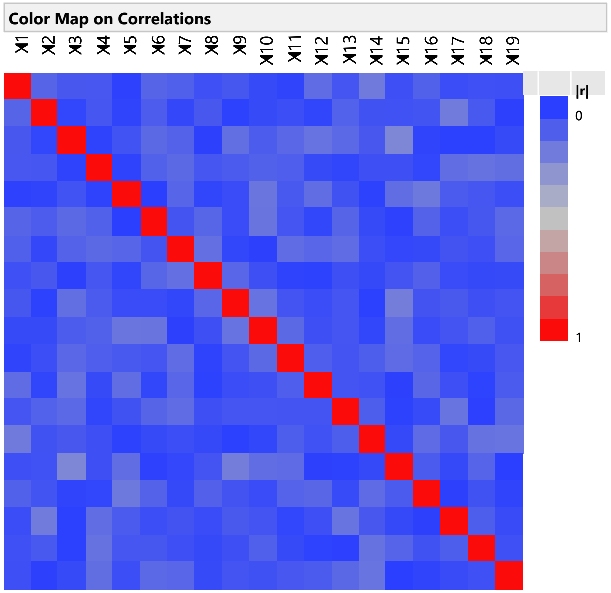
- **These are implemented in R package *MaxPro***



HOW MANY SIMULATIONS?

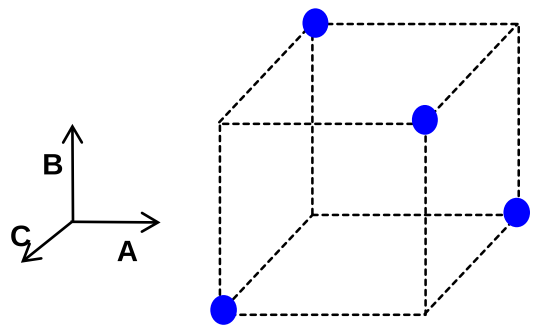
- **Generally, the rule of thumb for # of simulations in space-filling designs (Loeppky, Sacks, Welch, 2009) is 10*d**
- **Some recent work (Ba, Myers, Wang, 2018) seeks to exploit sequential experimentation to generate sensitivity analysis-derived weights**
  - These weights enable systematic augmentation (fold-over) using fewer MaxPro LHD runs in total
  - Still between 5-8 runs per dimension
- **For our 19 factor problem these approaches still give us between 95-190 simulations – infeasible given our 25-run budget**
- **Even MaxPro has trouble estimating effects with less than 5 runs per dimension**

19 factors in 57 runs (3*d)

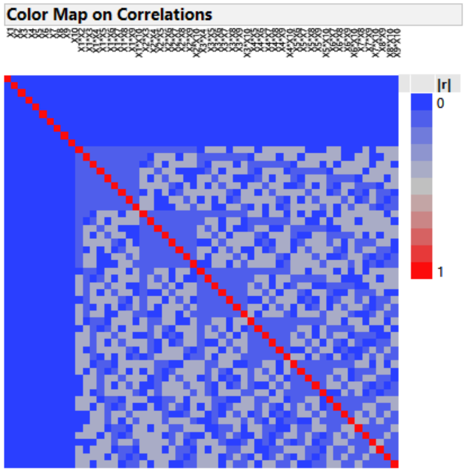


LET'S CONSIDER SOME ALTERNATIVES

- **Fraction-Factorial Designs**
  – We can capture gross trends/sensitivities for up to 15 factors in 16 runs (min = d+1)
  – Unfortunately, we can only count by 2^(k-p), increments don't easily allow for 25-run design
  – Bad projection for interior of design space, but good in terms of sample size efficiency



- **Definitive Screening Designs**
  – 2*d+1 runs
  – Main effects orthogonal to each other and two-factor interactions
  – Estimable quadratic effects (often complex M&S surfaces will be missed)
  – Lack desirable projection properties; don't form a dense set in entire design space, point redundancies



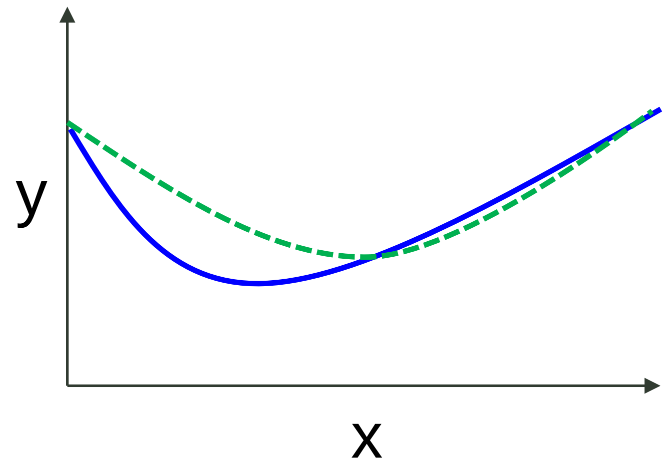
- **Optimal Designs**
  – Most flexible, any # of runs, different types of variables

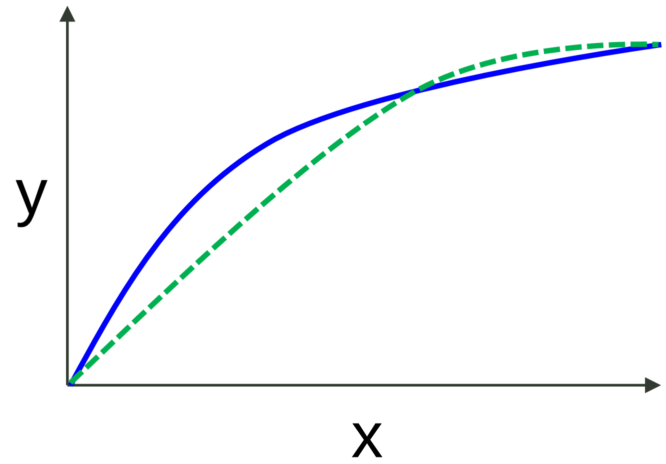
CURVATURE

- **Even very simple curvilinear function approximation using a second-order polynomial (green dashed line) can be mischaracterized**

- **Subtle differences (such as asymmetry) between the shape of the curve and how it is approximated results in systematic bias, inaccuracy in certain regions of the design space**

- **3-level designs such as DSD’s and optimal designs are not a good use of simulations in many cases, and the curvature is not known prior to fitting the data**



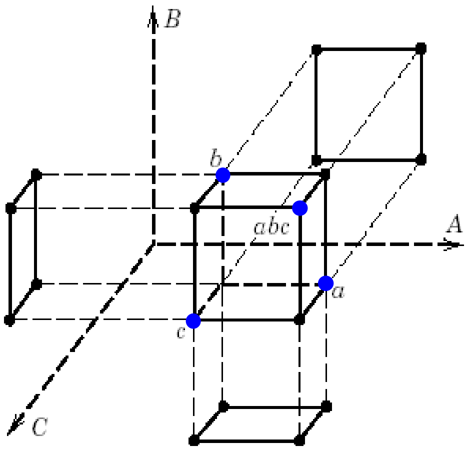


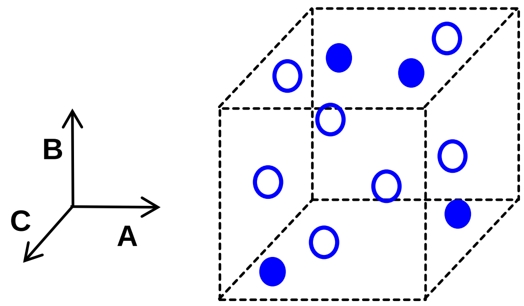
IDEA

- **What if we could *blend* the projection properties (and sample size) of a Fraction-Factorial or a D-optimal design with the space-filling properties of a LHD (such as Maximin or MaxPro)?**

- **Conceptually, we could use a probability distribution to 'dither' points around the corners of the design space, but enough into the interior to potentially capture nonlinearities in projection**

- **Generalized Maximin Latin Hypercube Design (G-MLHD) (Dette, Pepelshyev, 2011)**
  - Uses the arc-sin transformation (beta distribution with alpha=beta=0.5) to ensure asymptotic D-optimality for each projection, shifting points towards boundaries
  - Decent projection properties, but some limitations - does not ensure D-optimality of the design as a whole





D-LHD: BASIC CONCEPT

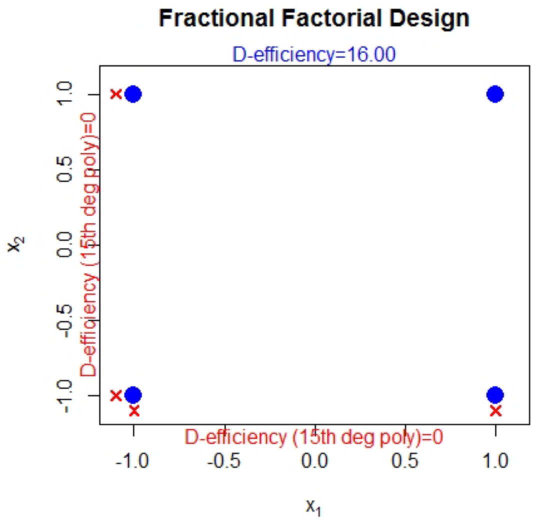
- **(Proposed) D-Optimal Latin Hypercube Design (D-LHD) (Joseph, Krishna, Ray, 2019)**
  - Blended design that combines the most desirable properties of factorial designs and space filling designs
  - Improvement in D-efficiency from the Generalized Maximin LHD using a coordinate exchange algorithm
  - Good projection properties

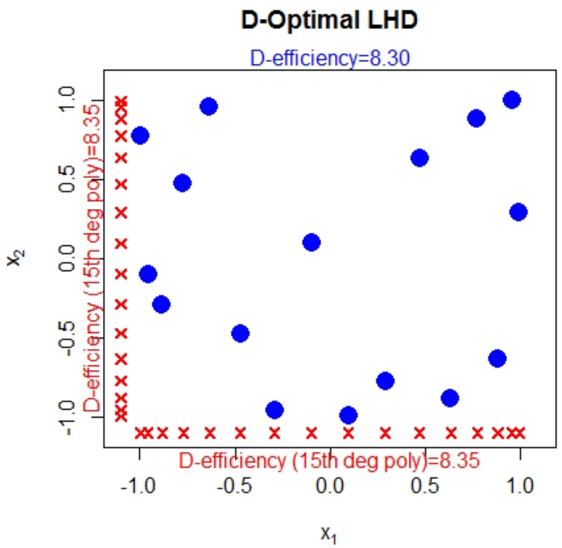
- **The proposed DLHD in n-runs is obtained by maximizing the D-efficiency of fitting a full linear main effects model within the class of LHDs, where the levels of the LHDs are chosen to maximize the one-dimensional D-efficiency (for fitting an n-1 degree polynomial).**
  - G-MLHD does not ensure D-optimality of the design as a whole
  - Overall D-optimality of G-MLHD can be improved by using a coordinate exchange algorithm
  - Coordinate exchange algorithm exchanges design coordinates along a design projection such that D-efficiency of the design increases

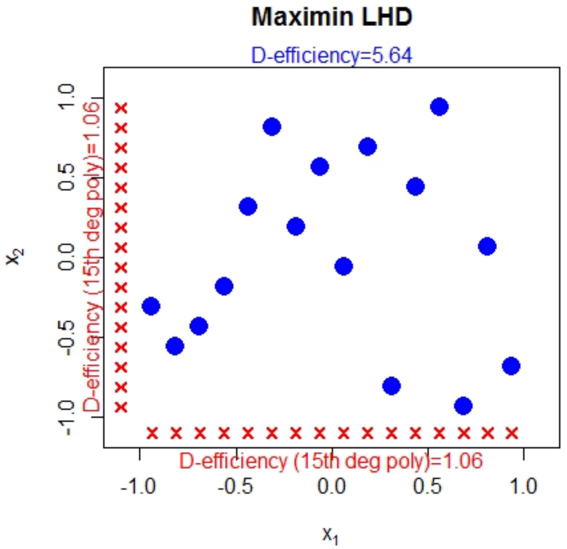
	Design			
Runs	X1	X2	X3	X4
1	0.8	0.4	0.6	0.3
2	0.7	0.9	0.4	0.0
3	0.9	0.5	0.7	0.1
4	0.3	0.1	0.5	0.4
5	0.2	0.6	0.7	0.0
6	0.7	0.8	0.1	0.5
7	0.5	0.8	1.0	0.4
8	0.9	0.0	0.3	[illegible]

D-LHD: BASIC CONCEPT (CONT.)

- **Three different designs, each with 15 factors in 16 runs:**
  1. FFD has the maximum D-efficiency for estimating a full linear main effects model (D-efficiency=16), but it has poor projections. If only one factor is significant, we could fit a 15-degree polynomial for which its D-efficiency is 0 (in fact, it is 0 even for fitting a quadratic polynomial).
  2. For the MmLHD, D-efficiency for a full linear main-effects model is 5.64 and has one-dimensional D-efficiency for fitting a 15-degree polynomial of 1.06.
  3. For the proposed D-optimal LHD, the D-efficiency for the full linear main effects model is 8.30 and has one-dimensional D-efficiency for fitting a 15-degree polynomial is 8.35. Thus, although its full model D-efficiency is not as good as that of an FFD, it has good D-efficiency if only a few factors are active. Clearly the D-efficiency of DLHD is better than that of MmLHD, so it is expected to perform better in screening.







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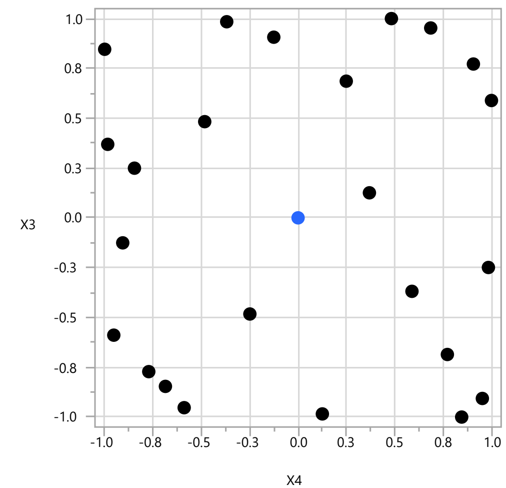
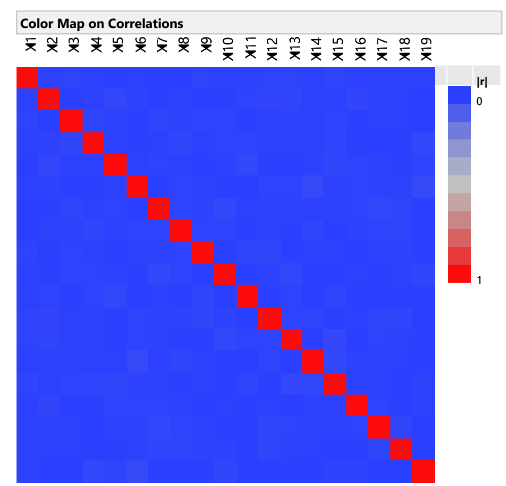
D-LHD DESIGN SPACE PROJECTION

- **The motivation for the D-LHD came from both problems where simulations are limited due to computing time, as well as highly-dimensional problems**

- **Let us consider an engineering problem with 40 factors**
  - We can explore this in as few as d+1 = 41 simulations, but much better results in 2*d+1 simulations (think DSD's)
  - A good approach to ID basic sensitivities, main effects
  - Augment significant factors with MaxPro for accurate prediction and optimization
  - Alternative is either 400 runs, or loss of information that comes with a three-level design

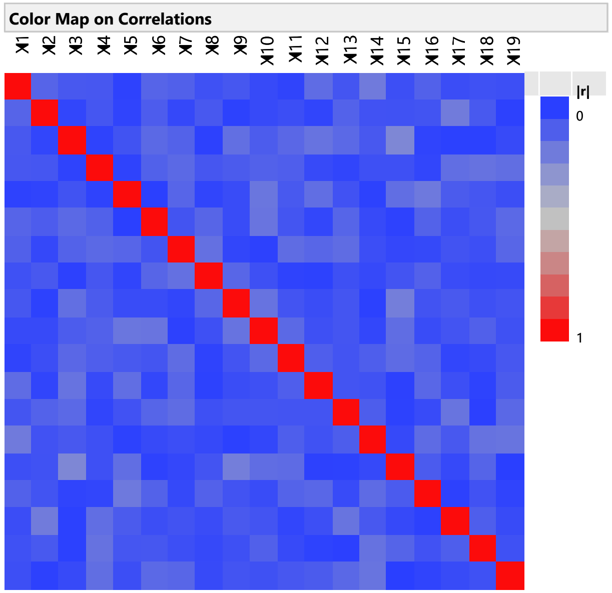
19 factors in 25 runs



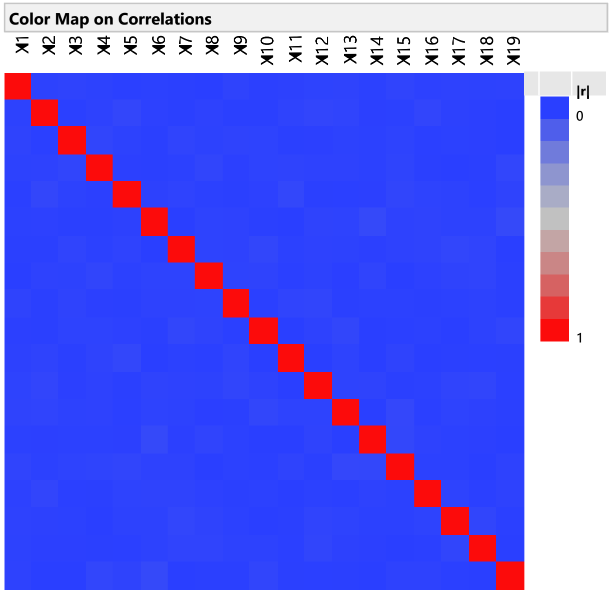


D-LHD VS. MAXPRO – 19 FACTOR EXAMPLE

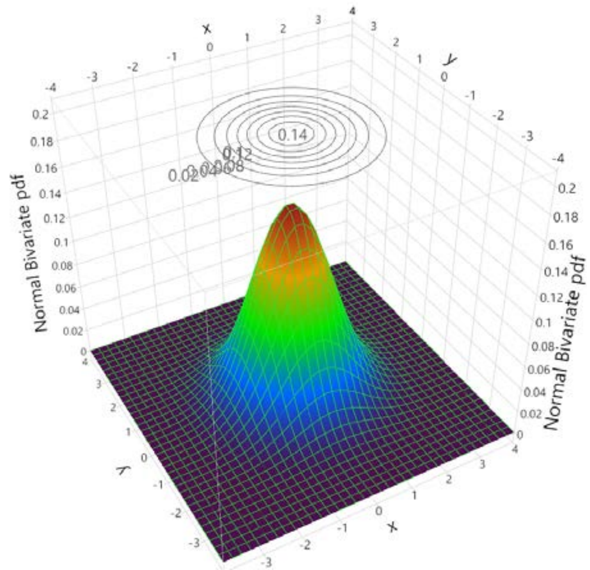
MaxPro: 57 runs (3*d)



D-LHD: 24+1C runs (1.3*d)

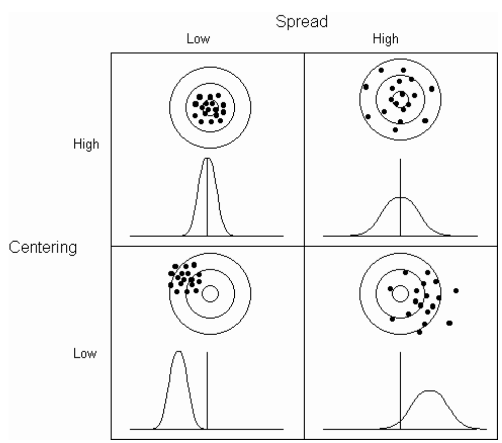


- **The concept of sequential experimentation leveraging design projection is not a new one, but for computer experiments it can be just as important as with physical experiments!**
- **Sequential experimentation = smarter investment in resources**

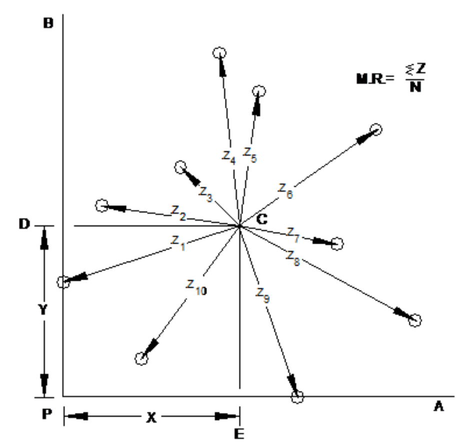


Case Study:

Small-Caliber Ammunition Dispersion M&S Study

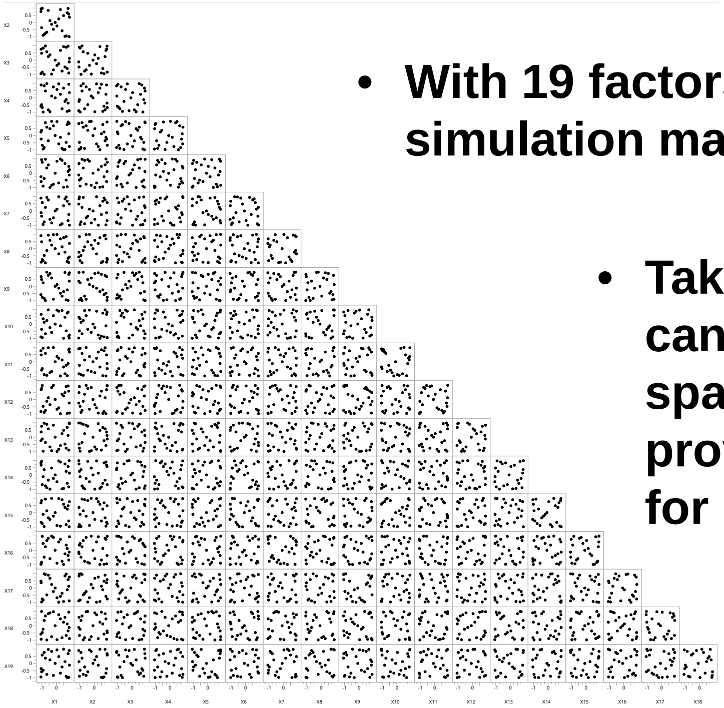


(http://syque.com/quality_tools/toolbook/Variation/measuring_variation.htm)



TEST DESIGN

- A multidisciplinary planning effort determines factors of interest for study
- D-LHD developed through a partnership between Statistical Sciences Group and Professor V. Roshan Joseph of Georgia Tech, the M&S screening design approach was inspired by these types of problems



- With 19 factors and 25 available runs, team generated simulation matrix used in the study
- Taking a closer look at the scatterplot matrix, we can see the points favoring the exterior of the space for enhanced D-efficiency, while also providing dense projection properties desirable for deterministic M&S statistical models

ANALYSIS

- The data was fit using a Gaussian Process model in JMP 13 Pro without the use of Fast GASP
- The empirical model showed promising results, with reasonable confidence bounds and findings that largely corroborated SME hypotheses
- In order to rank and order the variables by overall importance with respect to dispersion performance, JMP's variable importance platform was leveraged

Overall

Column	Main Effect	Total Effect
X8	0.184	0.232
X12	0.117	0.204
X3	0.11	0.133
X6	0.081	0.124
X14	0.103	0.117
X15	0.064	0.074
X13	0.026	0.053
X7	0.034	0.046
X5	0.035	0.044
X9	0.028	0.041
X16	0.015	0.03
X10	0.008	0.011
X19	0.004	0.009
X18	0.002	0.005
X1	0.001	0.003
X4	0.002	0.002
X11	0.001	0.002
X2	1e-17	2e-17
X17	1e-17	2e-17

Y1

Column	Main Effect	Total Effect
X8	0.34	0.394
X6	0.13	0.178
X12	0.043	0.135
X5	0.103	0.124
X14	0.076	0.086
X3	0.055	0.065
X7	0.049	0.059
X15	0.028	0.035
X10	0.025	0.033
X4	0.005	0.007
X11	0.001	0.002
X1	2e-17	2e-17
X2	2e-17	2e-17
X9	2e-17	2e-17
X13	2e-17	2e-17
X16	2e-17	2e-17
X17	2e-17	2e-17
X18	2e-17	2e-17
X19	2e-17	2e-17

Y2

Column	Main Effect	Total Effect
X12	0.307	0.477
X14	0.234	0.264
X13	0.078	0.159
X9	0.084	0.123
X8	0.029	0.094
X6	0.026	0.053
X18	0.007	0.015
X5	0.003	0.007
X1	1e-17	2e-17
X2	1e-17	2e-17
X3	1e-17	2e-17
X4	1e-17	2e-17
X7	1e-17	2e-17
X10	1e-17	2e-17
X11	1e-17	2e-17
X15	1e-17	2e-17
X16	1e-17	2e-17
X17	1e-17	2e-17
X19	1e-17	2e-17

Y3

Column	Main Effect	Total Effect
X3	0.275	0.332
X8	0.183	0.207
X15	0.163	0.188
X6	0.086	0.142
X16	0.045	0.089
X7	0.053	0.078
X19	0.013	0.027
X1	0.004	0.01
X11	0.002	0.005
X2	7e-18	2e-17
X4	7e-18	2e-17
X5	7e-18	2e-17
X9	7e-18	2e-17
X10	7e-18	2e-17
X12	7e-18	2e-17
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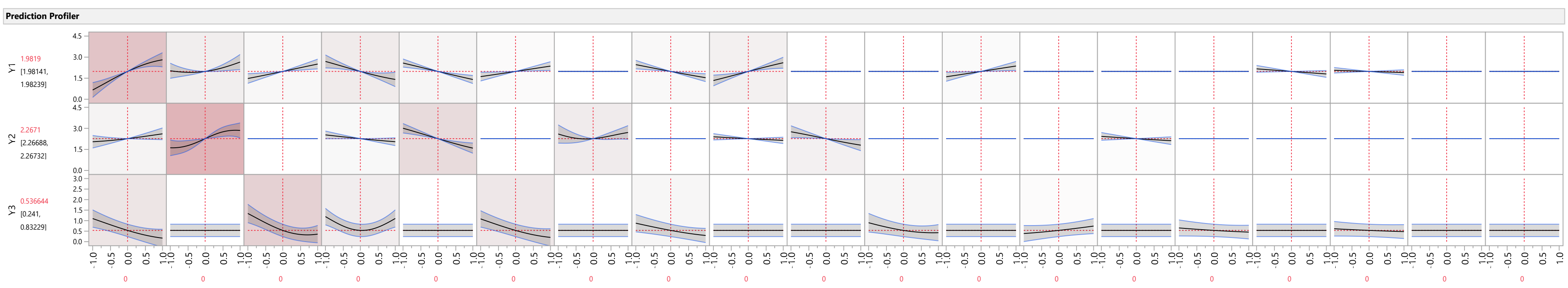
X17	7e-18	2e-17
X18	7e-18	2e-17



CONCLUSIONS & FUTURE WORK

- **For resource constrained M&S experiments, alternative methods to one-shot space filling experiments may be necessary**
  - Sequential D-LHD[1]
  - Sequential MaxPro methods[8]
  - Generalized Maximin LHD[9]

- **For simulation experiments where screening of factors is the primary initial objective, D-Optimal Latin Hypercube Designs provide the highest D-efficiency while maintaining desirable projection properties**

- **Augmentation of the D-LHD can supplement the experiment if further investigation into sparse or volatile regions of the space is required**

- **The first practical application of this method successfully helped Army engineers identify the most influential factors of a new bullet design with respect to dispersion performance**
  - Looking to future work, the team will explore the possibility of augmentation
  - The team is also working towards live testing to externally validate the model

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QUESTIONS