SAND2011-4889C

Progress Towards Nested Space and Sub-Space Filling Latin Hypercube Sample Designs

Keith Dalbey, PhD

Sandia National Labs, Dept 1441

Optimization & Uncertainty Quantification

George N. Karystinos, PhD

Technical University of Crete, Dept of Electronic & Computer Engineering

July 25 – July 28, 2011

Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy's National Nuclear Security Administration under Contract DE-AC04-94AL85000.

Sandia National Laboratories

Outline

- Sampling: Why & What's Good?
- Sample Design Quality Metric: Centered L2 Discrepancy
- "Binning Optimality," a New Space-filling Metric
- Latin Hypercube Sampling (LHS)
- Jittered Sampling
- Binning Optimal Symmetric Latin Hypercube Sampling (BOSLHS)
- Nested Sub-Space Filling BOSLHS
- Conclusions
- Current / Ongoing Work

Sampling: Why & What's Good?

Problem: generate a M dimensional sample design with N points at which to evaluate a simulator

Why sample simulator input?

- To calculate statistics of outputs with uncertain inputs
- To optimize e.g., guess several times and pick best guess
- To construct meta-models (fast surrogates for slow simulators)

What qualities do we want in a sample design?

- Design should be **space-filling**
- **Low-dimensional projections** of points should be **well spaced**
- Sample point locations should be uncorrelated with each other
- **Regularity is bad**, leads to biased results
- **Nesting**: want a SEQUENCE of designs that inherit all points from earlier members in the sequence

Sample Design Quality Metric: Centered L2 Discrepancy

- Lots of metrics; fortunately one of them is almost always the most important
- **"Discrepancy"** (some norm of difference between points per sub-volume and uniform density)**: lower is better**
  - "Koksma-Hlawka-like inequality" bounds error in a computed mean in terms of discrepancy
  - **Centered L2 Discrepancy (usually most important metric)**
  - Wrap-Around L2 Discrepancy (important for periodic variables)
- Unfortunately, discrepancy is expensive ($O(M N^2)$ ops) to calculate for designs with large numbers of points, N, so...
- Can't guess a large number of designs & pick the best
- **WARNING: Regularity is easy way to get low discrepancy**

"Binning Optimality" a New Space-filling Metric

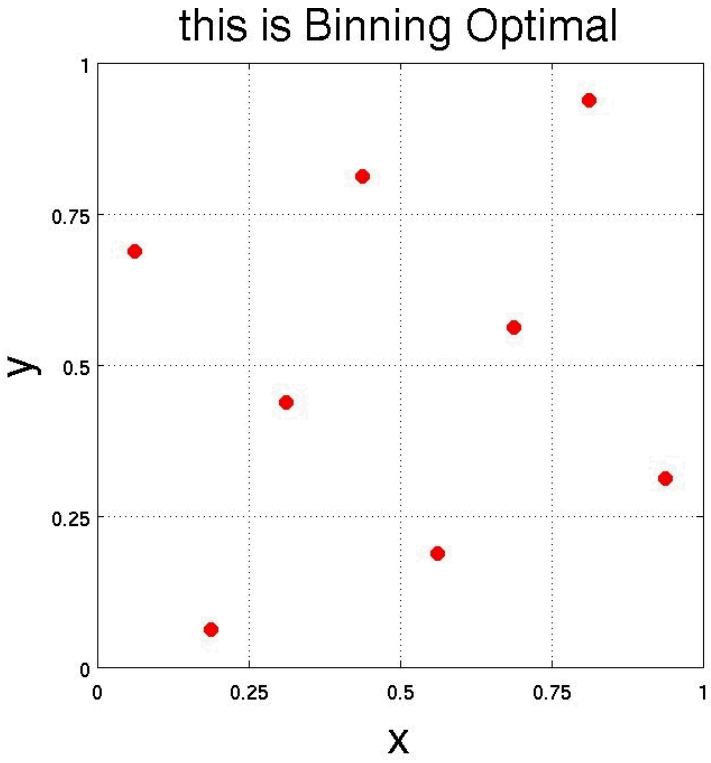
A sample design is "Binning Optimal" (in base 2) **if**

Short answer:

Every sub-bin that should contain a point does

Long answer:

- When you **recursively** subdivide M-dimensional hypercube into 2^M disjoint congruent sub-cube bins, all bins of same generation contain same number of points
- The above must hold true until bins are so small that they each contain either 0 or 1 points

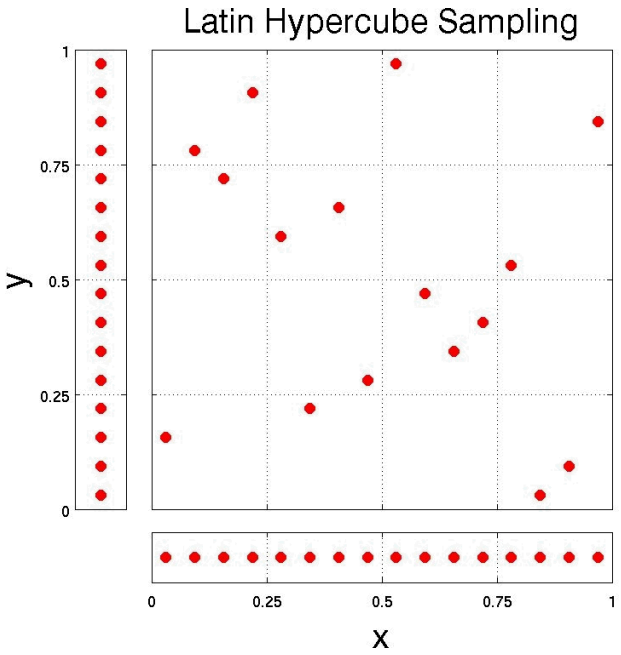


Sandia National Laboratories

Degree of Binning Non-Optimality...

...can be used to compare sample designs that are NOT binning optimal: Two numbers (g,s)

- "**g**" is the smallest # of **G**enerations above the smallest size bins at which all bins have the same # of points.
- "**s**" maximum # of points in any bin of the **S**mallest size.
- Can compare degree of binning non-optimality of all m-D subsets of dimensions for 1≤m≤M; an M by 3 array of numbers. The third number, "f" is the Fraction of m-D designs that are **not** binning optimal.

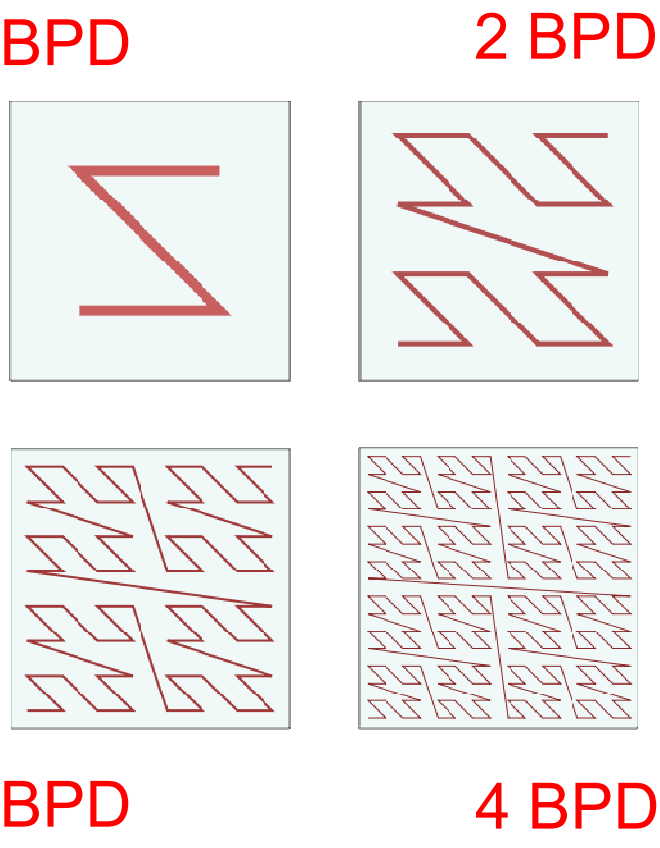


m	g	s	f
1	0	1	0
2	2	3	1

Sandia National Laboratories

Degree of Binning Non-Optimality Can Be Evaluated in O(N log(N)) Ops

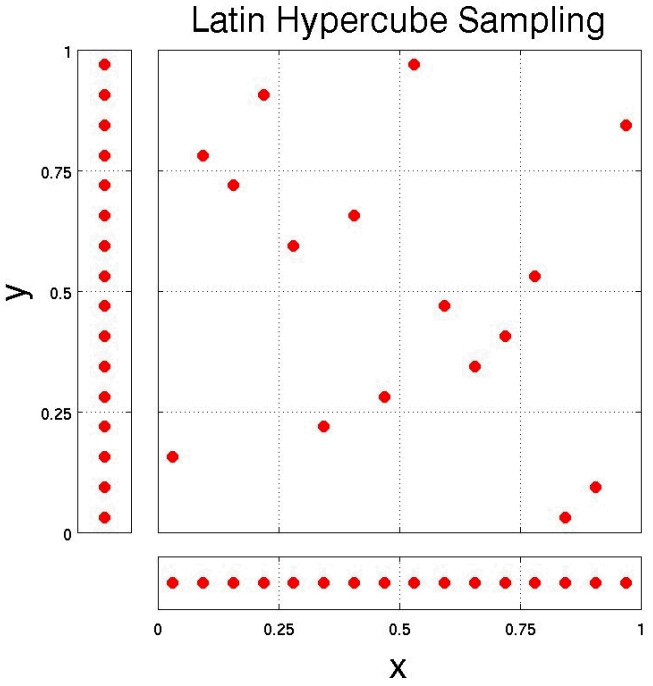
- Generate bin ids as indices into a Morton space-filling curve, also known as a "Z-curve." O(N log(N))+O(N M) work to collect leading Bits Per Dimension (BPD)
- Quicksort bin ids: O(N log(N)) work
- Tally bins ids: O(N) work



- A FFT of difference of sequential sorted Z-curve bin ids reveals regularity (cyclic patterns)

Latin Hypercube Sampling (LHS)

- Form of stratified random sampling that converges with fewer points than Monte Carlo Sampling
- Each column contains 1 point
- Each row contains 1 point
- **Quality** of design **depends on pairing of dimensions** used to form points (tough problem)
- Cell-centered LHS with randomly paired dimensions
  - **gets 1D projections "perfect"**
  - **is NOT space-filling**



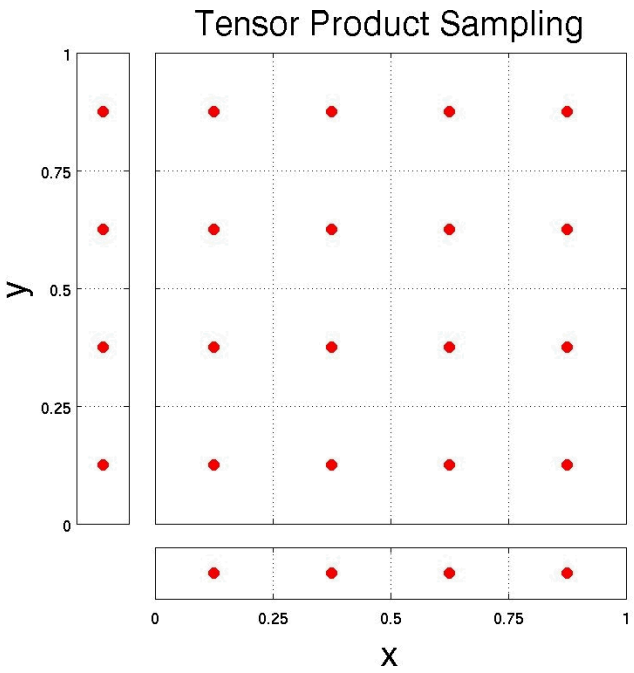
This is not Binning Optimal

m	g	s	f
1	0	1	0
2	2	3	1

Sandia National Laboratories

Jittered Sampling

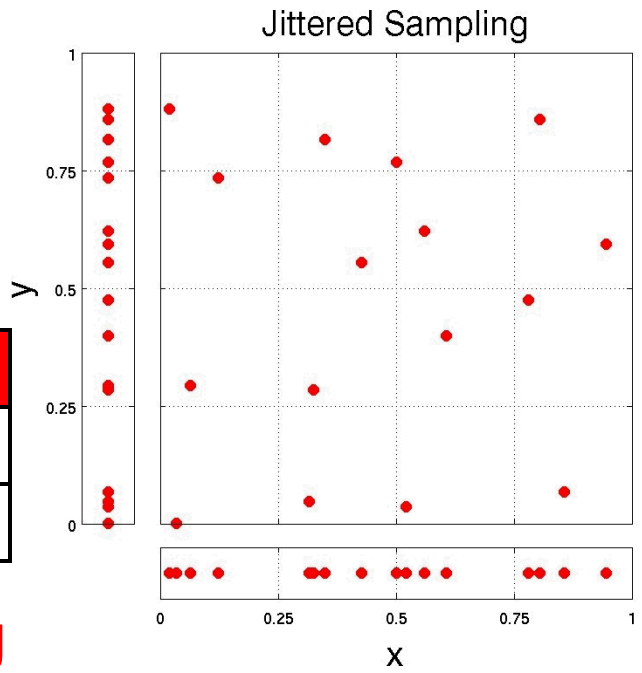
- Jittered Sampling = Tensor product sampling + random offset
- Better 1D projections than Tensor Product sampling
- **Worse 1D projections than LHS**
- Each cell contains a point $\Rightarrow$ **space-filling** as cell size $\rightarrow 0$



m	g	s	f
1	2	4	1
2	0	1	0

m	g	s	f
1	2	3	1
2	0	1	0

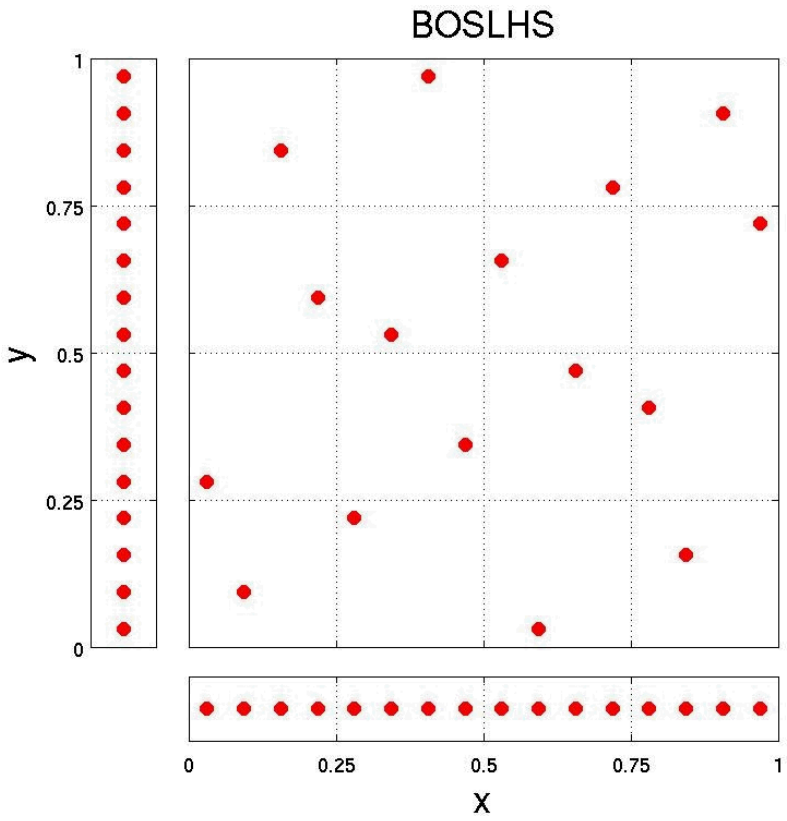
These are Binning Optimal



Sandia National Laboratories

Binning Optimal Symmetric Latin Hypercube Sampling (BOSLHS)

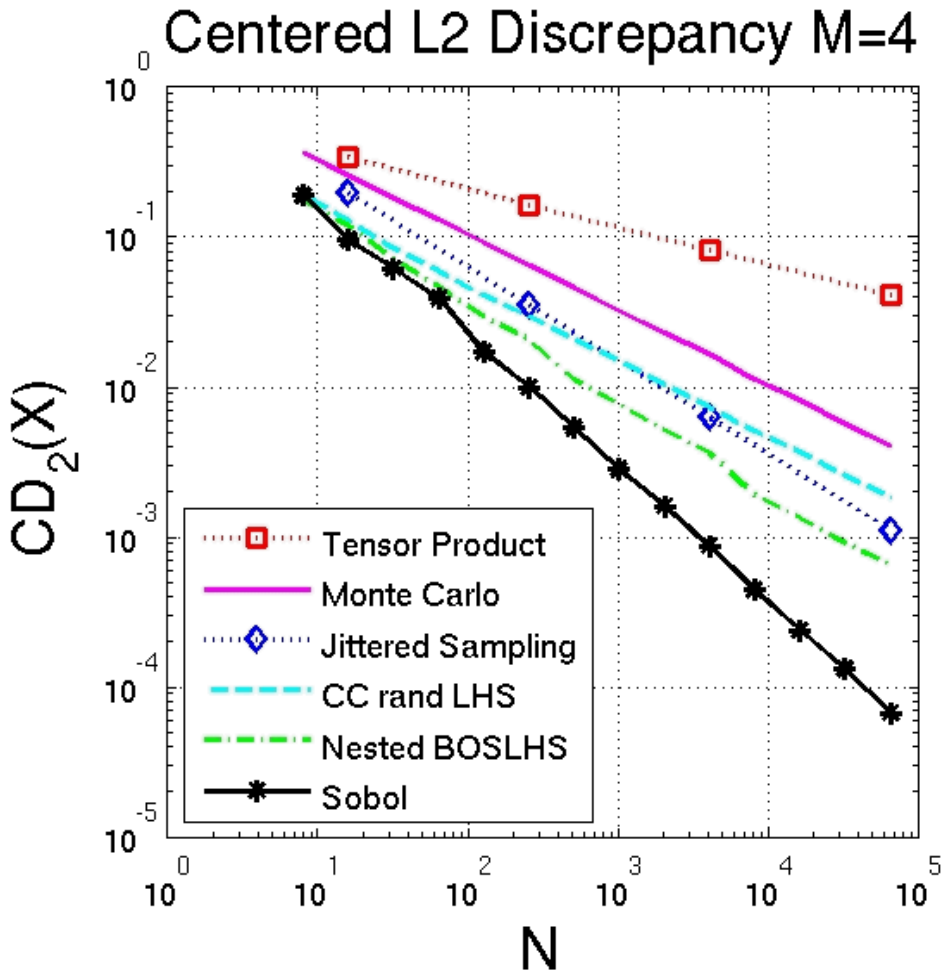
- Gets 1D projections right
- Is space-filling
- Combines most of best features of LHS and Jittered sampling
- Design quality is better than regular LHS or Jittered sampling
- Is **very** fast: generated **Nested** BOSLHS M=8 dim, $N=2^{16}=65536$ points design in 8.21 seconds
- Currently limited to $M=2^p \leq 16$ dimensions (low degree of binning non-optimality for non integer p, working on extending to $M > 16$)

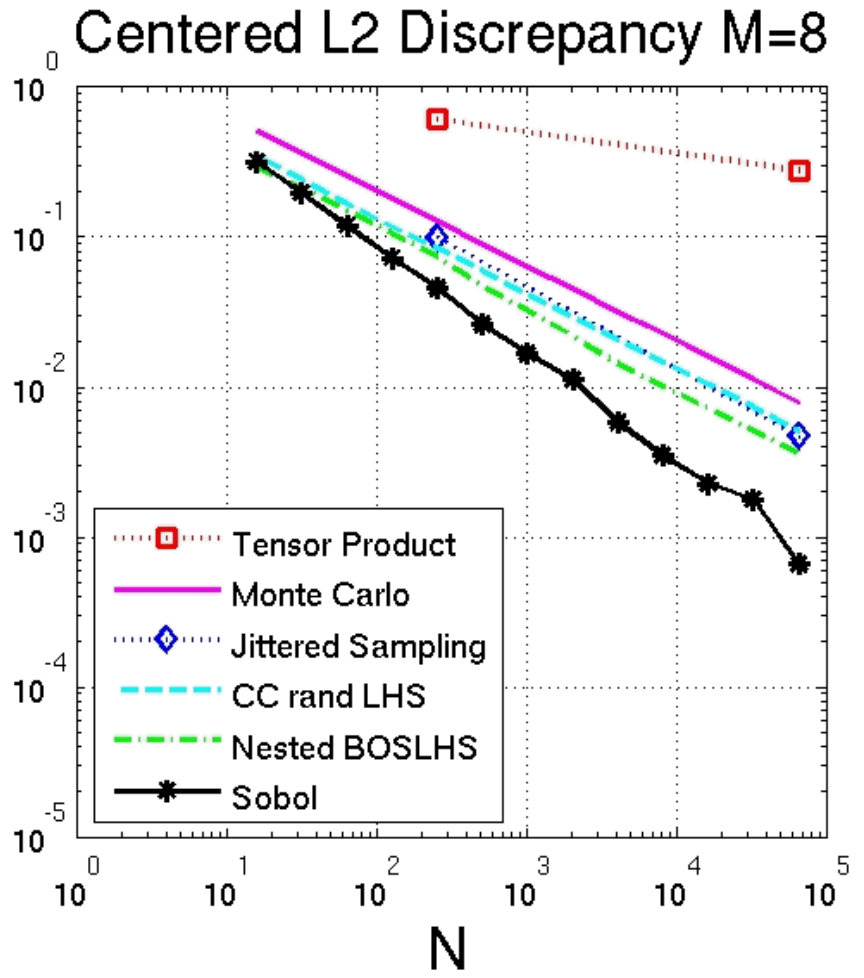


m	g	s	f
1	0	1	0
2	0	1	0

Sandia National Laboratories

How Does BOSLHS Compare With Other Methods: Centered L2 Discrepancy (Lower is Better)

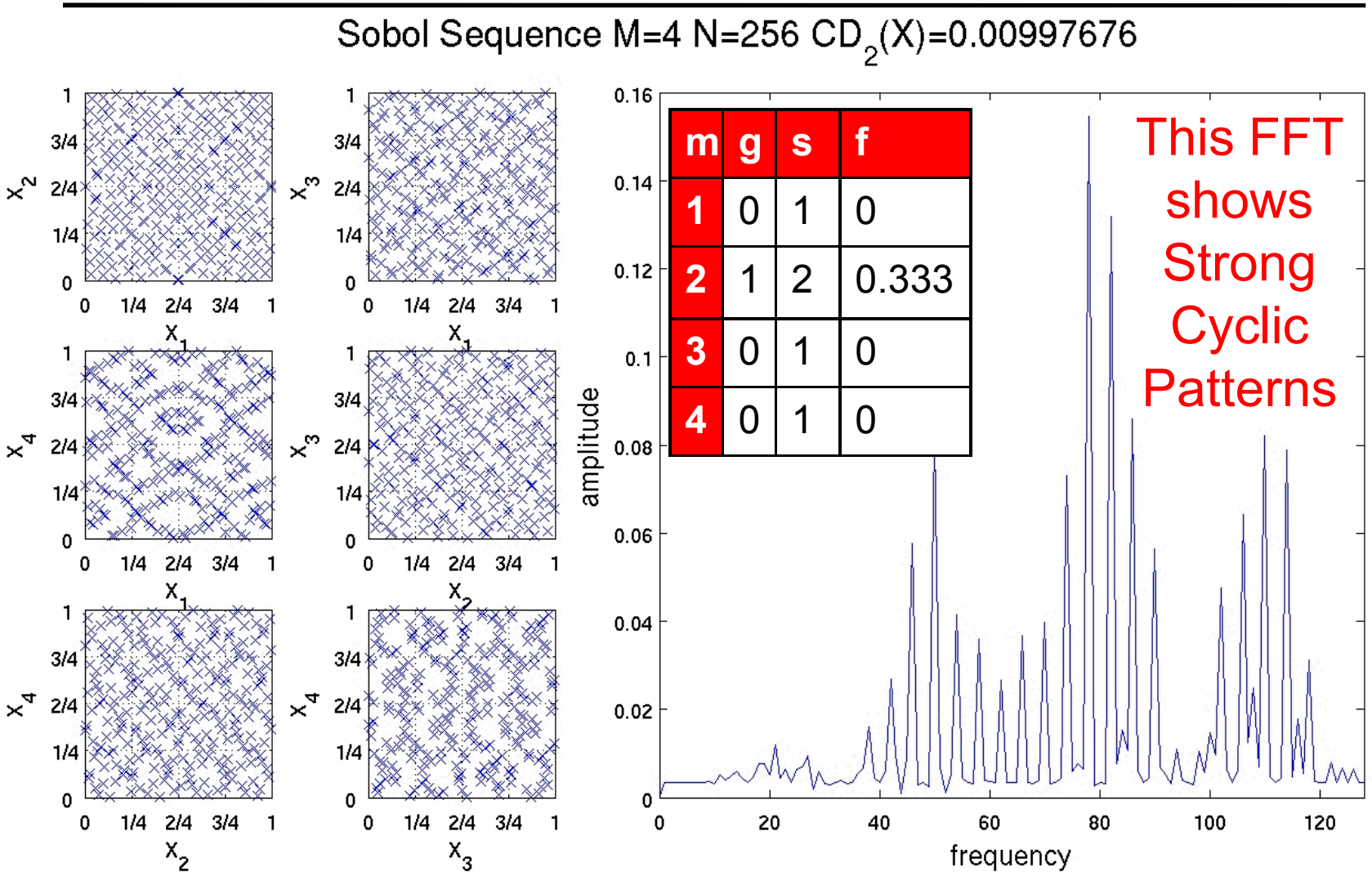




Plots are for average of 40 random designs

Sandia National Laboratories

The Sobol Sequence Has Lower Discrepancy But Is Regular



Regularity in sample designs results in biased statistics

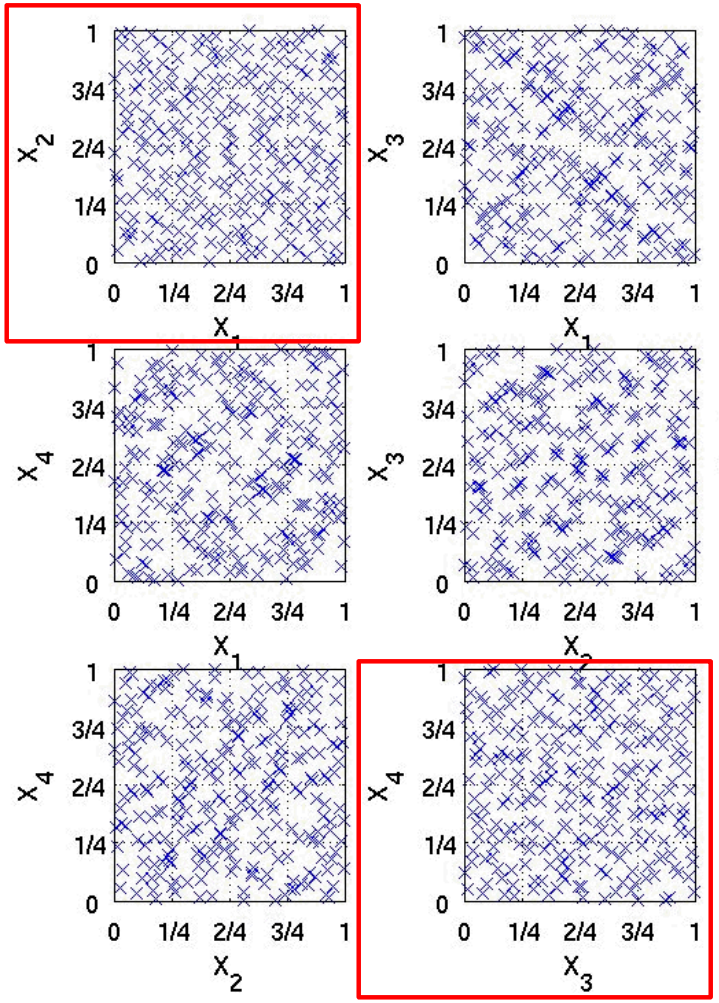
Sandia National Laboratories

Nested Sub-Space Filling BOSLHS

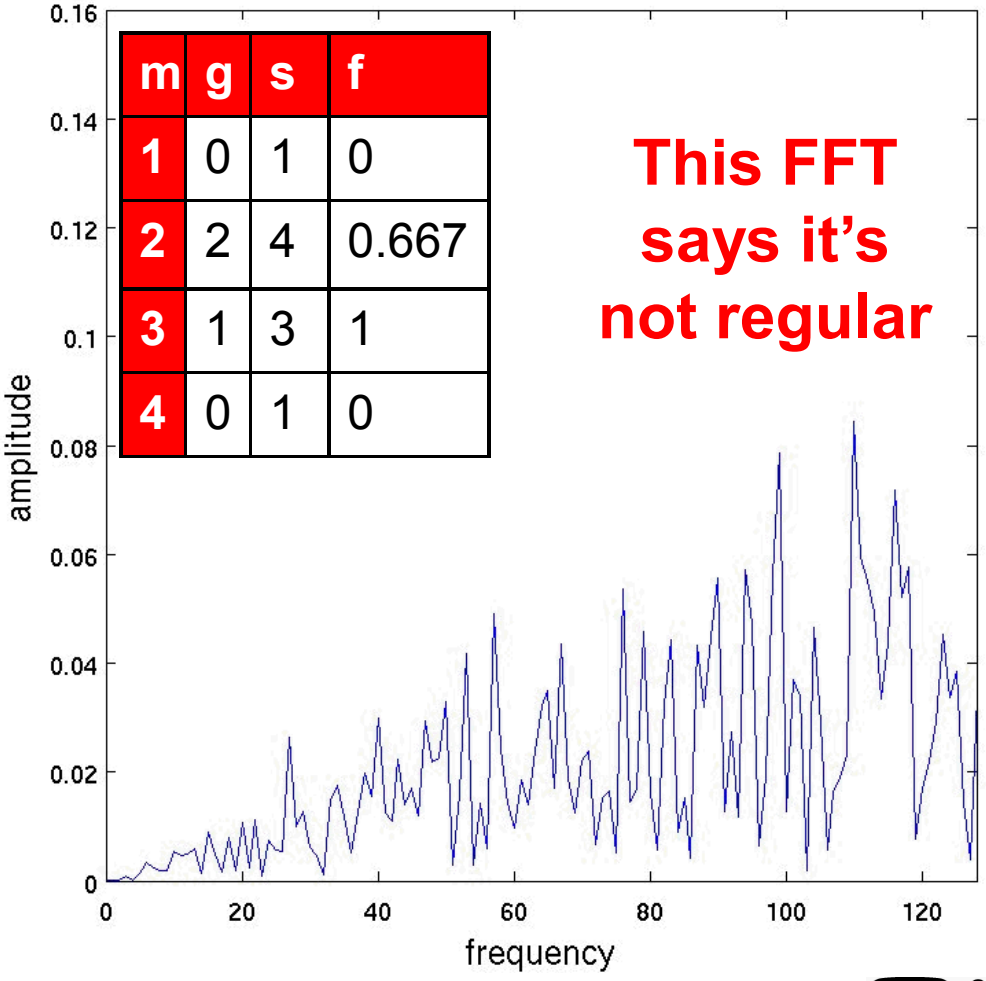
- Need to get leading ceil(log2(N)/m) BPD "right" to be binning optimal in m-dimensions
- m=1 is easy (Latin Hypercube Sampling)
- m=M=2^p (space filling) isn't too hard, just need a lists of which bins to fill in (Dalbey & Karystinos 2011)
- Other m (space and/or sub-space filling) are harder
- Also making it nested/inherited is harder still
- First cut was to randomly match first log2(N)/M BPD of M/2 2D BOSLHS designs to M-D design

First Cut of Nested Sub-Space Filling BOSLHS

M=4 N=256 Nested, First Cut Subspace Filling, BOSLHS $CD_2(X)=0.01634$



m	g	s	f
1	0	1	0
2	2	4	0.667
3	1	3	1
4	0	1	0



This FFT says it's not regular

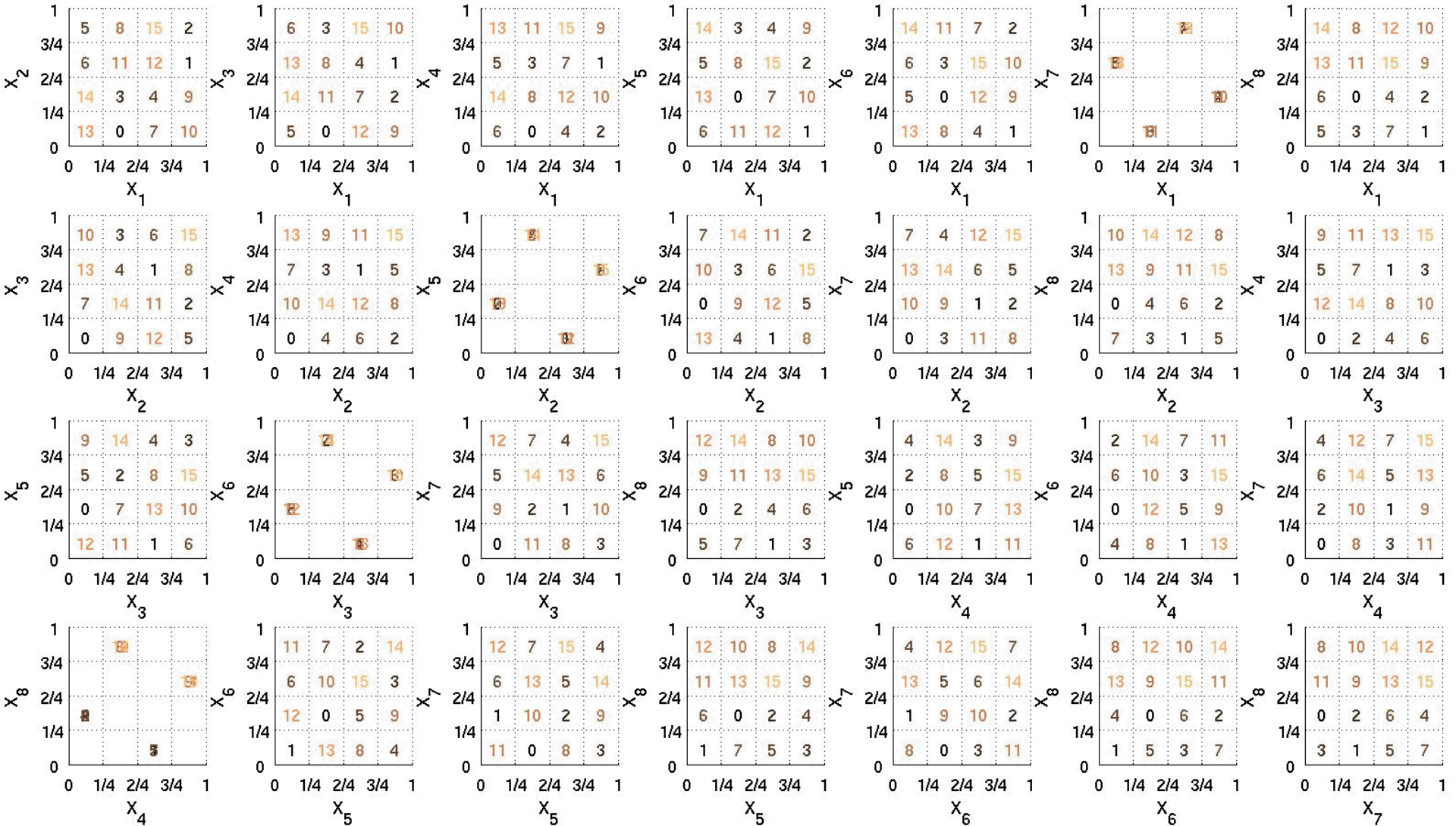
Sandia National Laboratories

Nested Sub-Space Filling BOSLHS

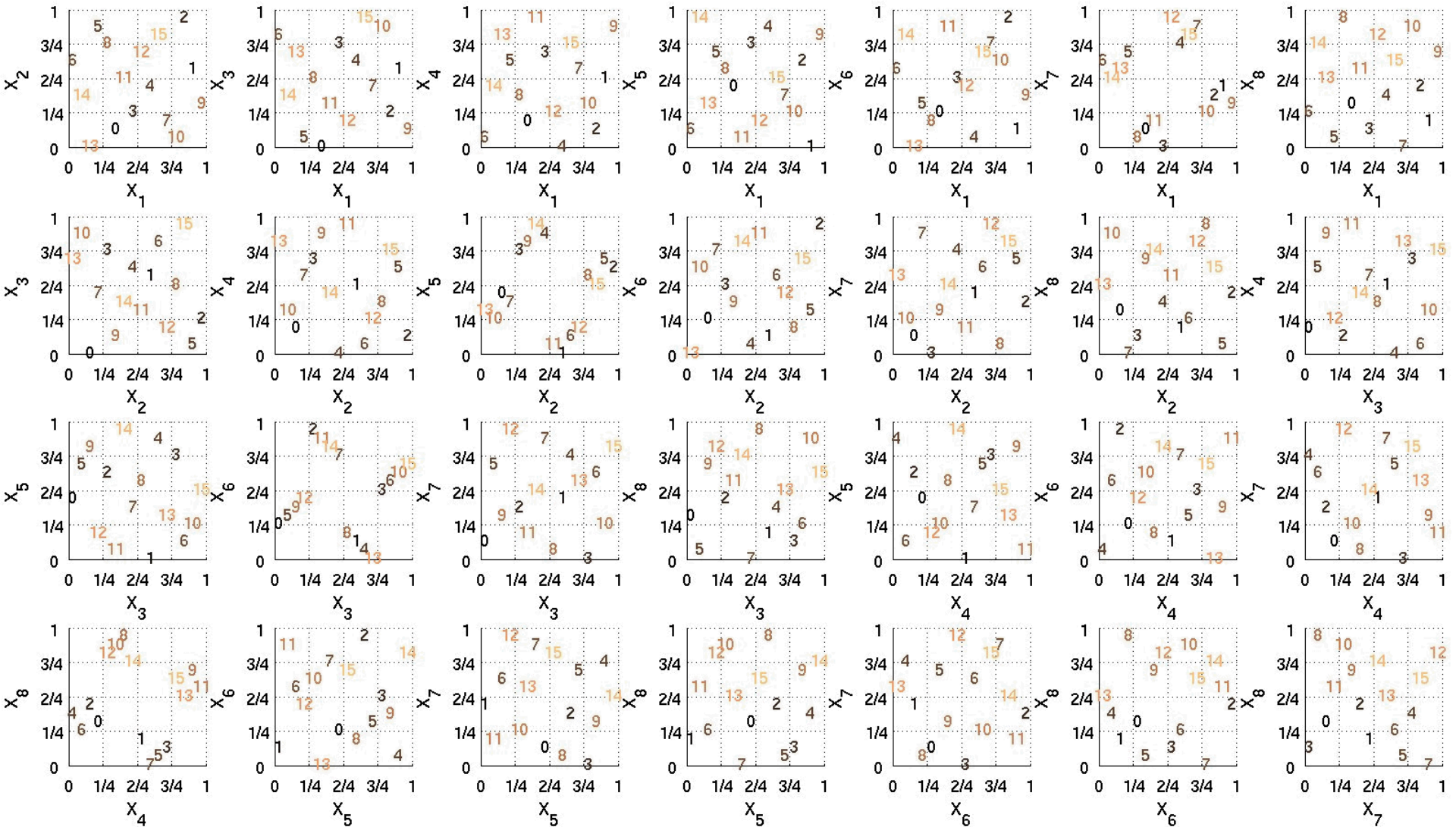
- Want binning optimality in more subsets of dimensions
- Good sub-space filling properties lets one discard dimensions and still have good space filling properties
- Ran into difficulties because of initial design (end points of a rotated orthogonal axis) in nested sequence.
- Need to keep leading BPD (from Sylvester construction of Hadamard matrices) to ensure it's still binning optimal but can change less significant BPD
- Undertaking "piecewise brute force" (use solutions from previous pieces to reduce work) examination of optimal starting designs

In 8D, an Optimal Choice of First 2 BPD

16 pts, 2 BPD, BOS design #1: $CD_2(X)=0.361915$ $(g_2,s_2,f_2)=(1,4,0.142857)$



Can Randomly Match First 2 BPD to 8 1D LHS designs to Make it BOSLHS



Previous 8D, 2 BPD, 16 Point Design

- Was 1 of 64 equivalent optimal designs found by brute force matching of 128 optimal 4D designs with leading BPD from 8D Sylvester Hadamard Matrix
- Was space-filling in all 3D, 5D, 6D, 7D, and 8D projections
- Was space-filling in 24/28 of 2D projections and 56/70 of 4D projections

m	g	s	f
1	2	4	1
2	1	4	0.1429
3	0	1	0
4	1	2	0.2
5	0	1	0
6	0	1	0
7	0	1	0
8	0	1	0

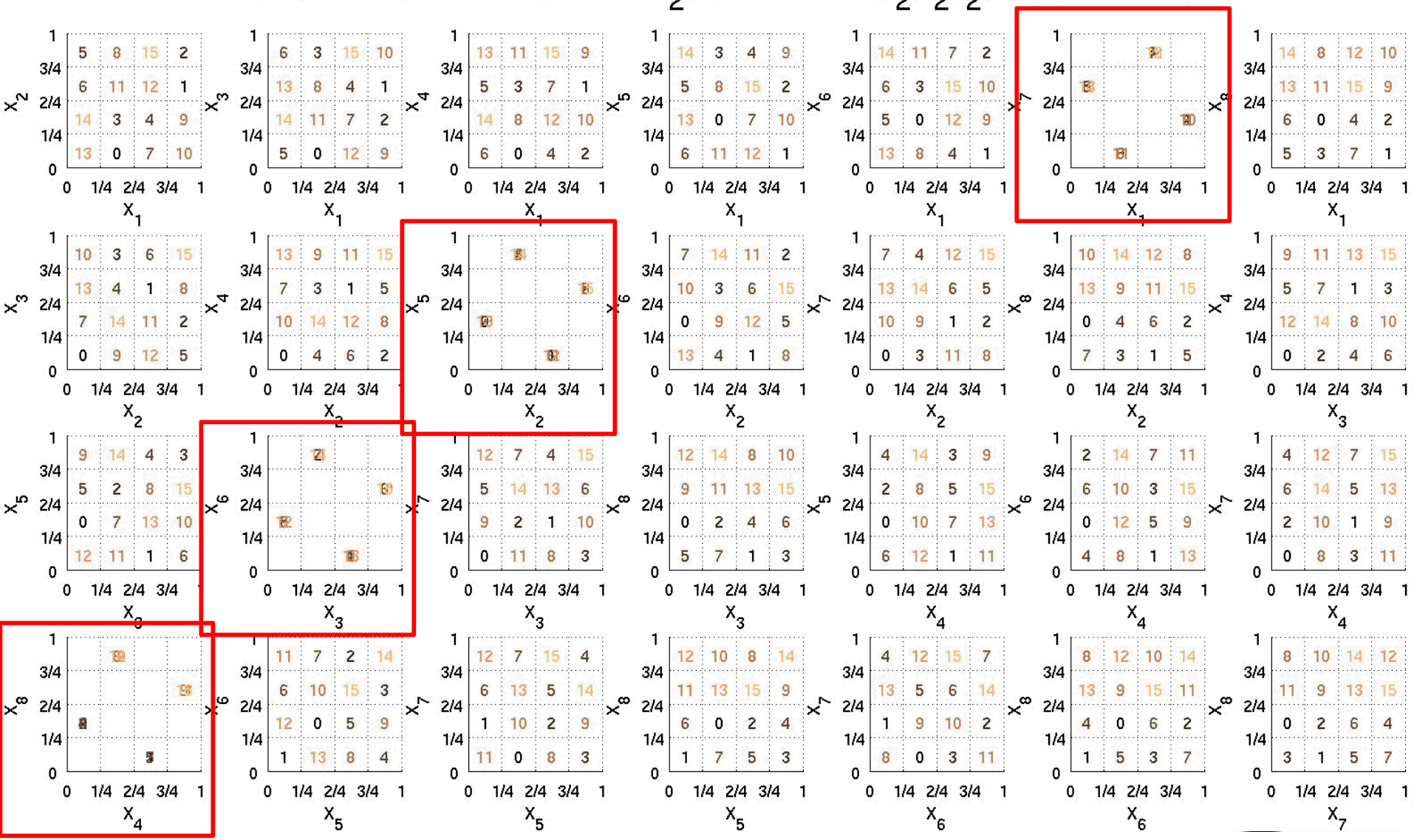
But there were other designs that differed in s_2, f_2, and centered L_2 discrepancy

- Notice that the # of equivalent designs, s_2, and f_2 are symmetric vertically
- Compare the next 4 designs, 2 were selected from the top group, 2 were selected from the bottom group

$CD_2(X)$	#Equiv	s_2	f_2
0.361915	64	4	0.142857
0.368682	192	3	0.571429
0.372019	512	4	0.357143
0.373236	512	3	0.571429
0.375327	192	2	0.428571
0.376533	1536	3	0.571429
0.379801	1536	3	0.571429
0.380993	1536	3	0.571429
0.381856	64	3	0.571429
0.383041	512	3	0.571429
0.384223	3072	3	0.571429
0.385402	512	3	0.571429
0.386577	64	3	0.571429
0.387427	1536	3	0.571429
0.388596	1536	3	0.571429
0.391763	1536	3	0.571429
0.392919	192	2	0.428571
0.394905	512	3	0.571429
0.396052	512	4	0.357143
0.399161	192	3	0.571429
0.405306	64	4	0.142857

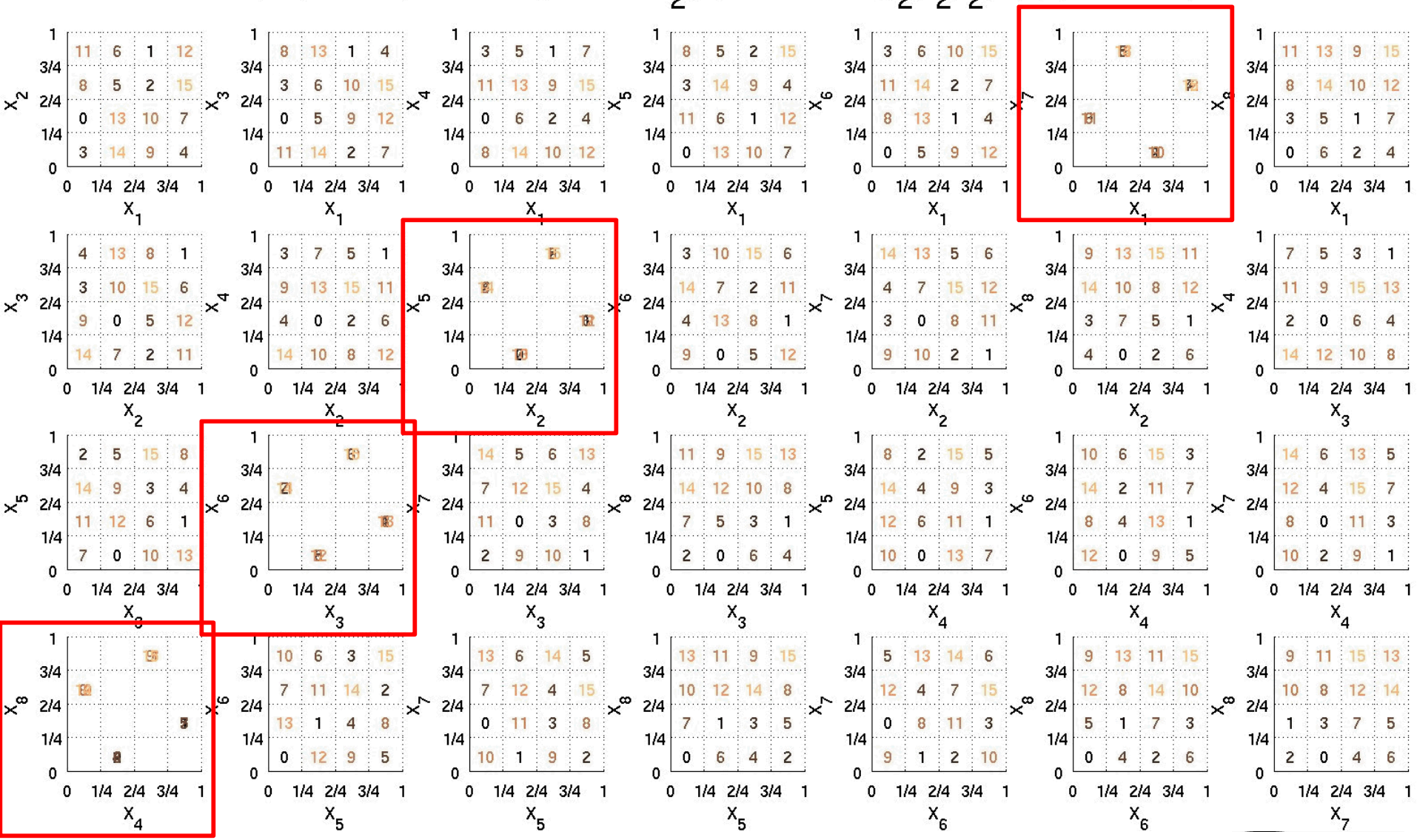
Design # 1 (Top Group)

16 pts, 2 BPD, BOS design #1: $CD_2(X)=0.361915$ $(g_2,s_2,f_2)=(1,4,0.142857)$



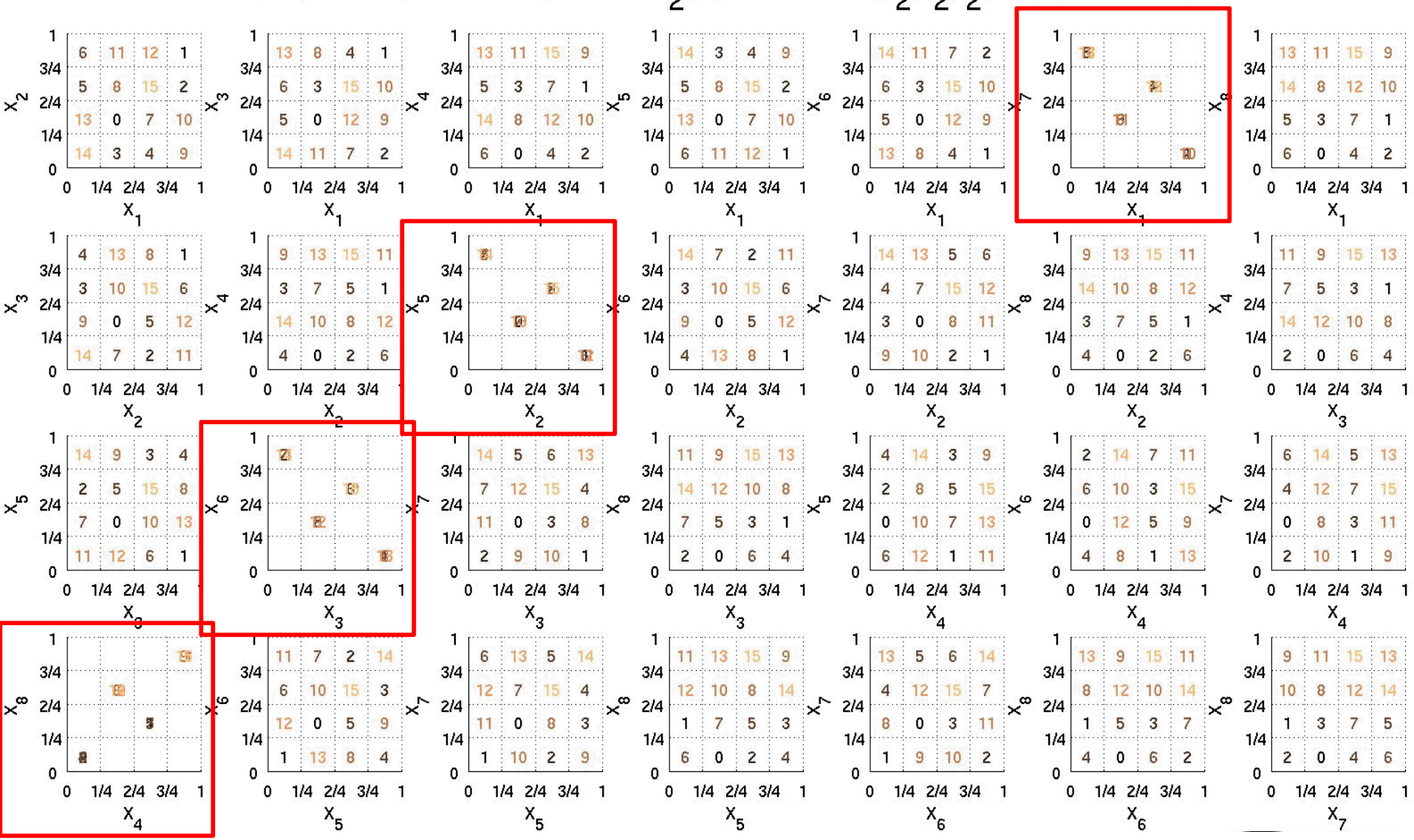
Design # 2 (Top Group)

16 pts, 2 BPD, BOS design #2: $CD_2(X)=0.361915$ $(g_2,s_2,f_2)=(1,4,0.142857)$



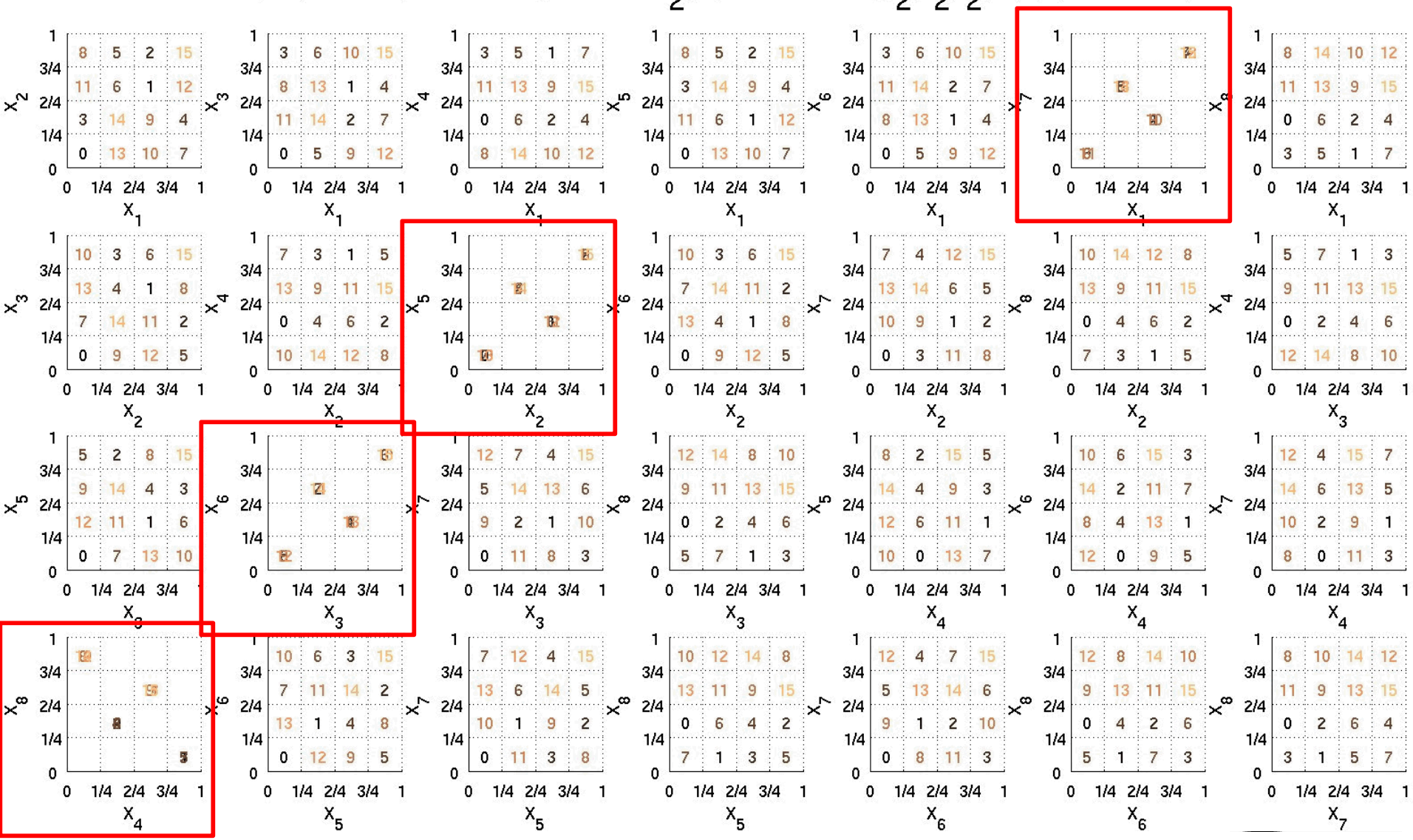
Design # 3 (Bottom Group)

16 pts, 2 BPD, BOS design #3: $CD_2(X)=0.405306$ $(g_2,s_2,f_2)=(1,4,0.142857)$



Design # 4 (Bottom Group)

16 pts, 2 BPD, BOS design #4: $CD_2(X)=0.405306$ $(g_2,s_2,f_2)=(1,4,0.142857)$



What Does This Mean?

It may be possible (and easy/fast) to

- start with a leading BPD design that is space-filling in the full M dimensional space and most subsets of dimensions,
- add matched leading BPD designs to evenly fill in “holes” to obtain a nested sequence of designs, and
- avoid regularity by randomly matching leading BPD with M one dimensional LHS designs

Conclusions

- Defined new space-filling metric "Binning Optimality" that evaluates in O(N log(N)) time
- Found related way to detect regularity in sample designs
- Developed fast algorithm for **Nested** Binning Optimal Symmetric Latin Hypercube Sampling (BOSLHS) that
  - **is also Binning Optimal in some Low D subsets**
  - combines best features of LHS & Jittered Sampling

Current / Ongoing Work

- Sub-space filling BOSLHS
- Extension to larger (> 16) and arbitrary (non power of 2) numbers of dimensions (sub-space filling BOSLHS could solve the latter)
- Better numerical quantification of “regularity”
- ? Induce correlations between dimensions?
- How well do emulators built from BOSLHS designs predict (paper submitted to Statistics & Computing)
- Gradient Enhanced Kriging emulators

References

1. K. R. Dalbey and G. N. Karystinos, “Fast Generation of Space-filling Latin Hypercube Sample Designs,” *Proceedings of the 13th AIAA/ISSMO Multidisciplinary Analysis and Optimization Conference, 2010.*

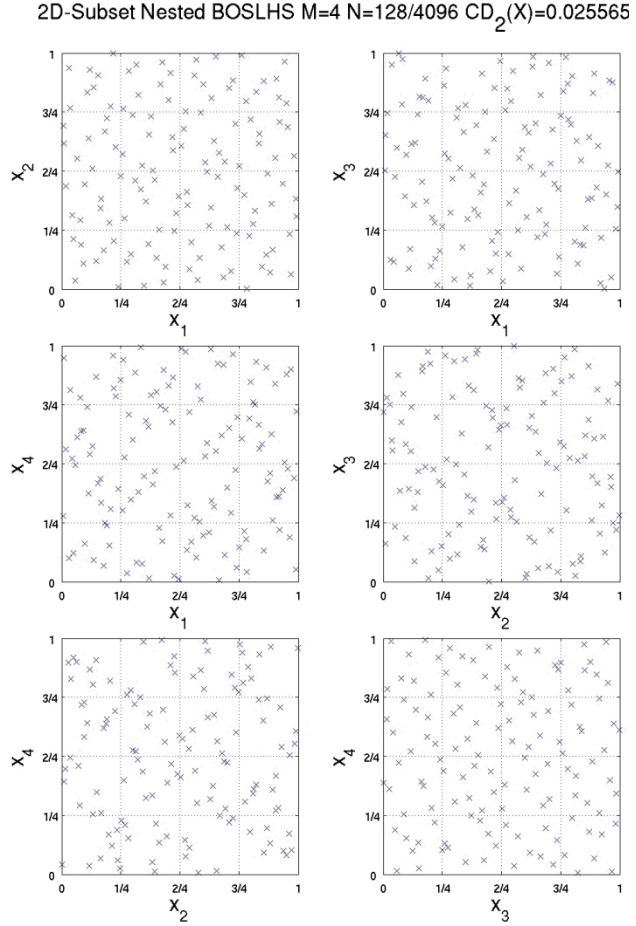
2. K. R. Dalbey and G. N. Karystinos, “Generating a Maximally Spaced Set of Bins to Fill for High Dimensional Space-filling Latin Hypercube Sampling,” *International Journal for Uncertainty Quantification*, vol. 1(3), pp. 241 - 255, 2011.

Bonus Slides Start Here

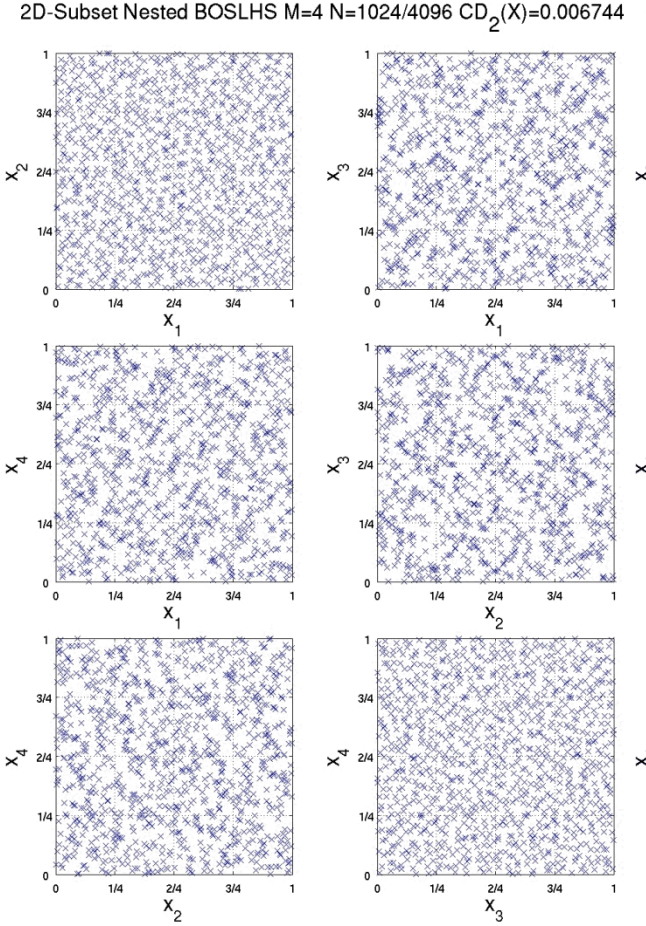
Sandia National Laboratories

First Cut Results (Dims 1&2, 3&4): Eyeball Metric M = 4D

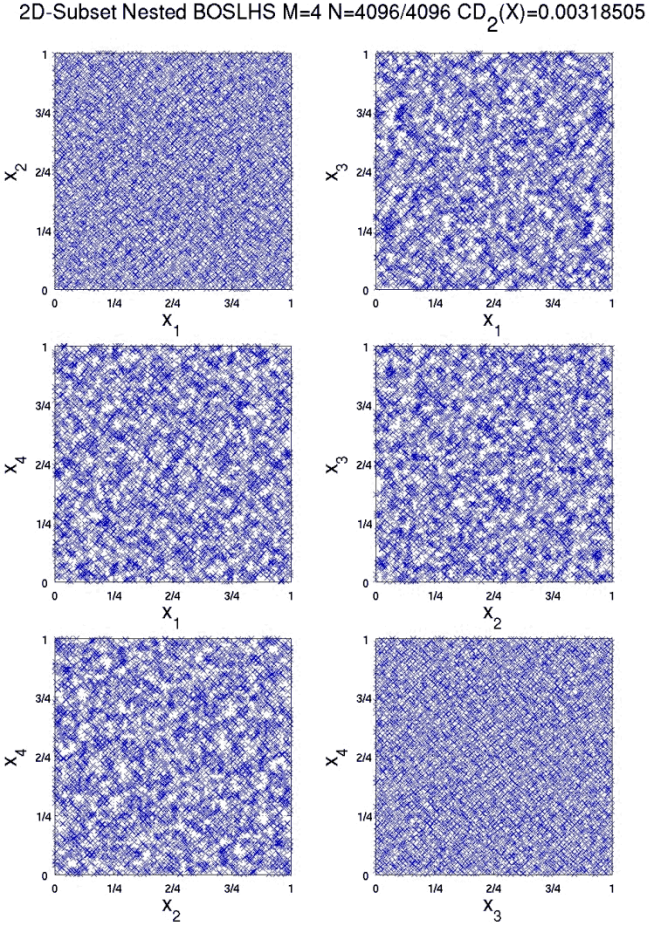
N=128



N=1024



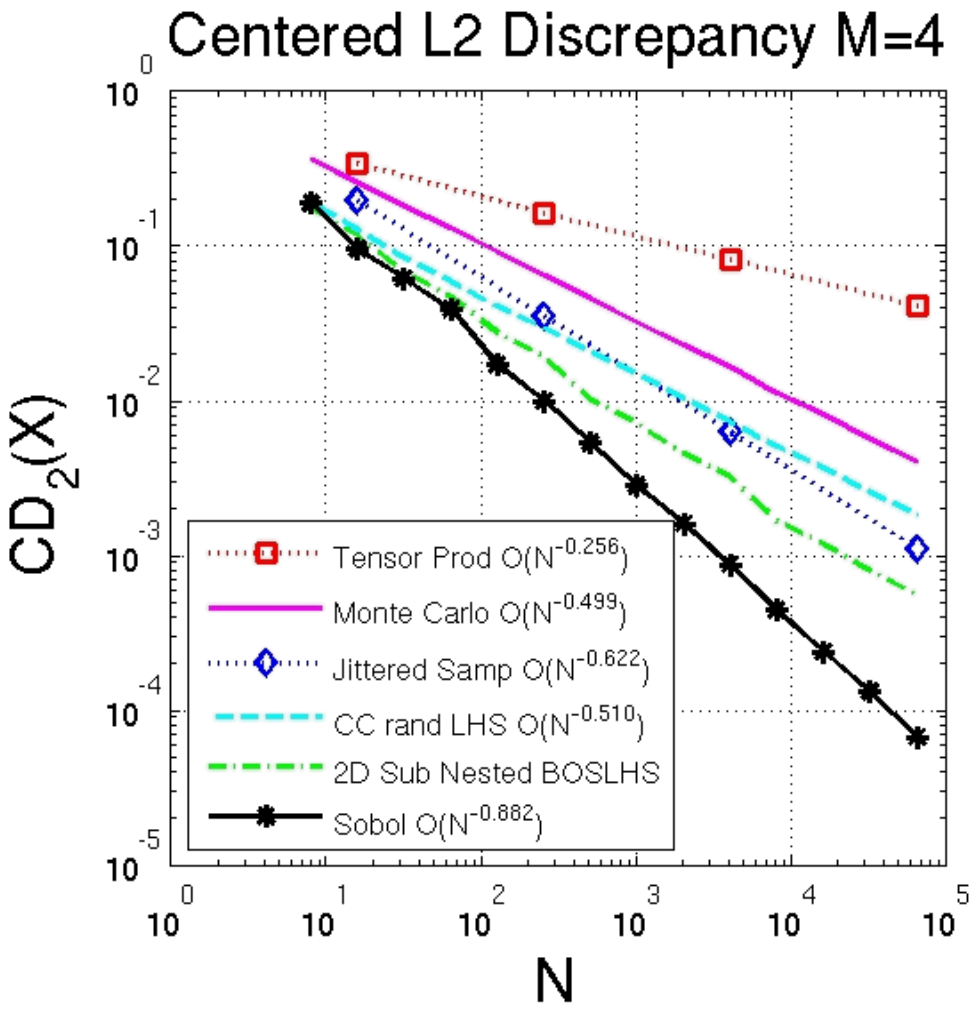
N=4096

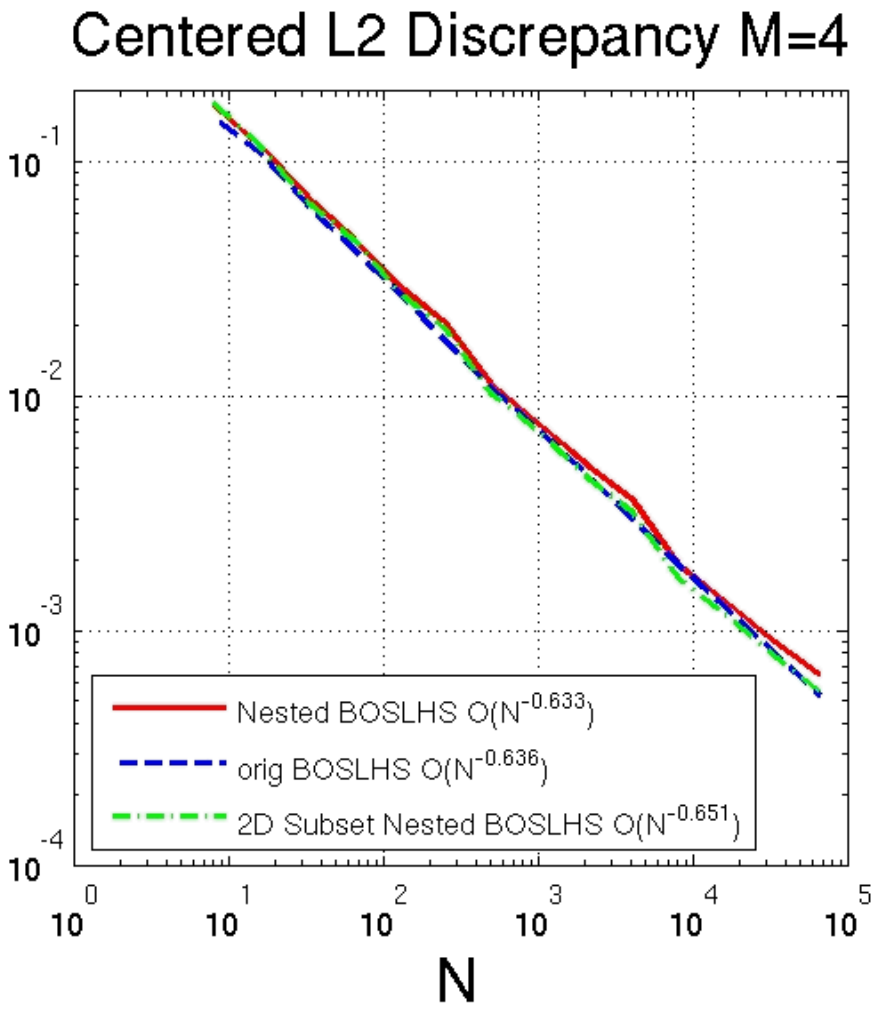


- Plotted all 6 combinations of 2 out of M = 4 dimensions
- BOSLHS is visibly space-filling!

Sandia National Laboratories

First Cut Results: Centered L2 Discrepancy (Lower is Better)

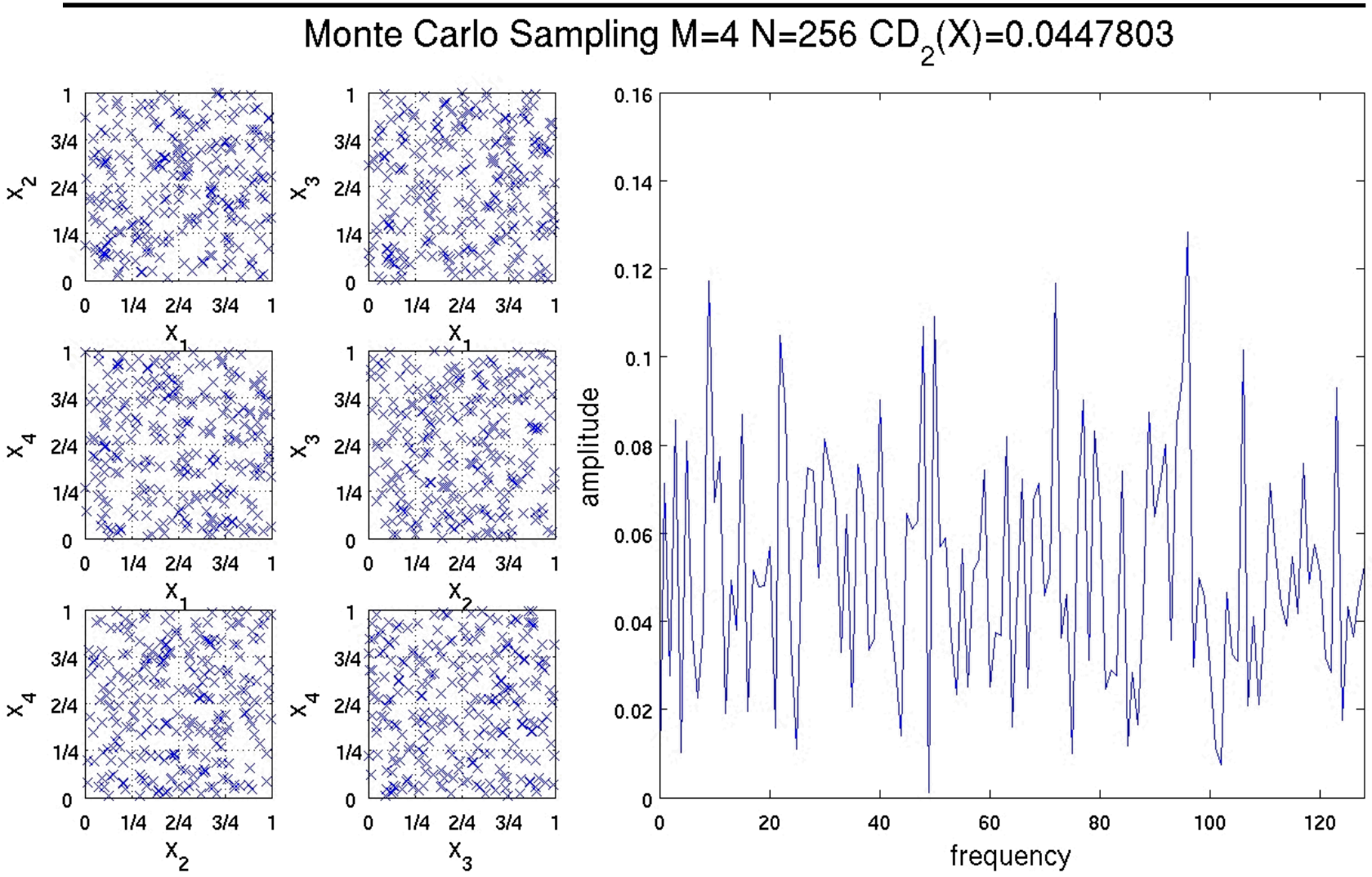




Plots are for average of 40 random designs

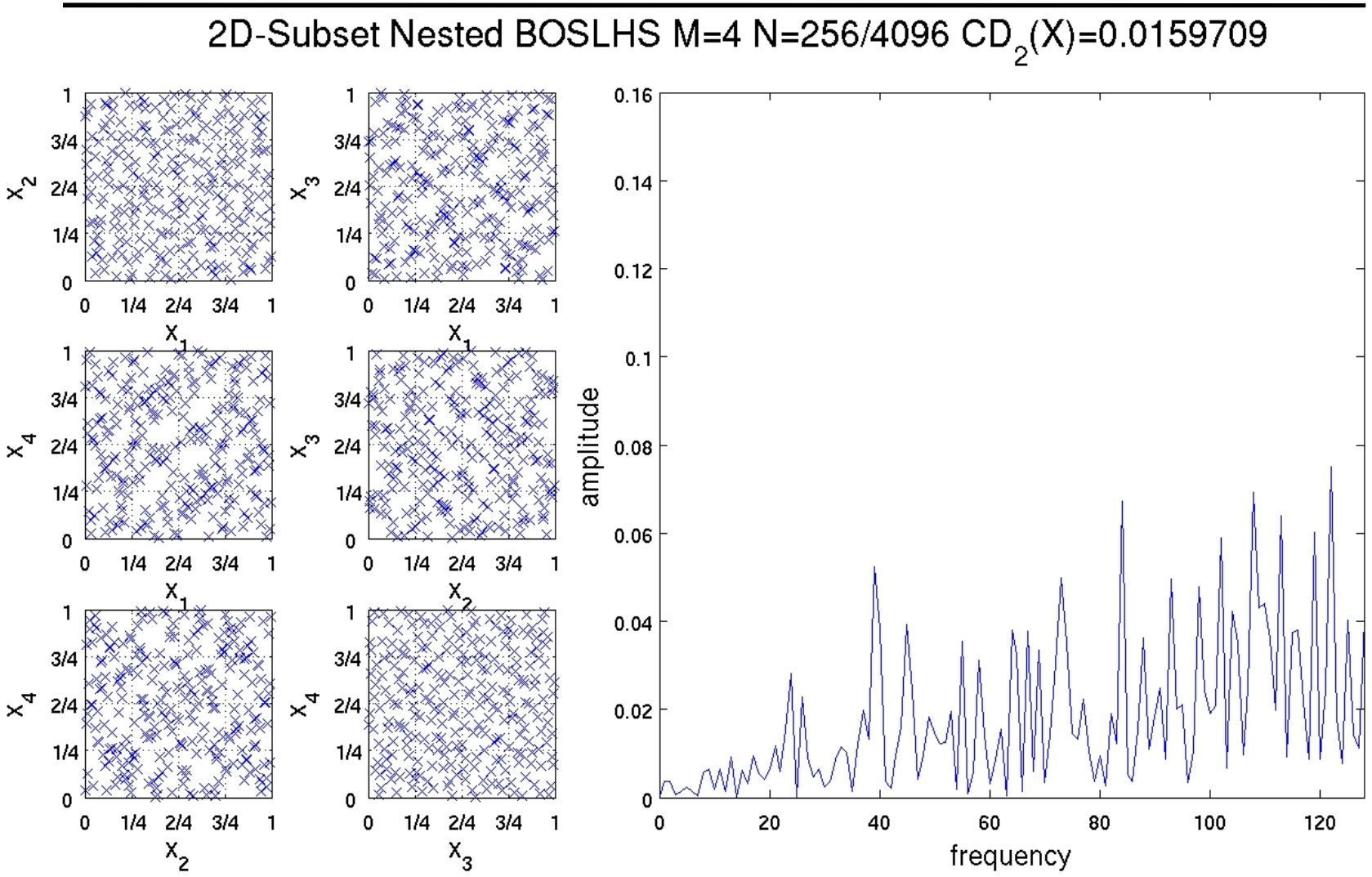
Sandia National Laboratories

Results: What Complete Irregularity (Monte Carlo Sampling) Looks Like



Sandia National Laboratories

First Cut Results: Nested BOSLHS Is Not Regular



Sandia National Laboratories

Results

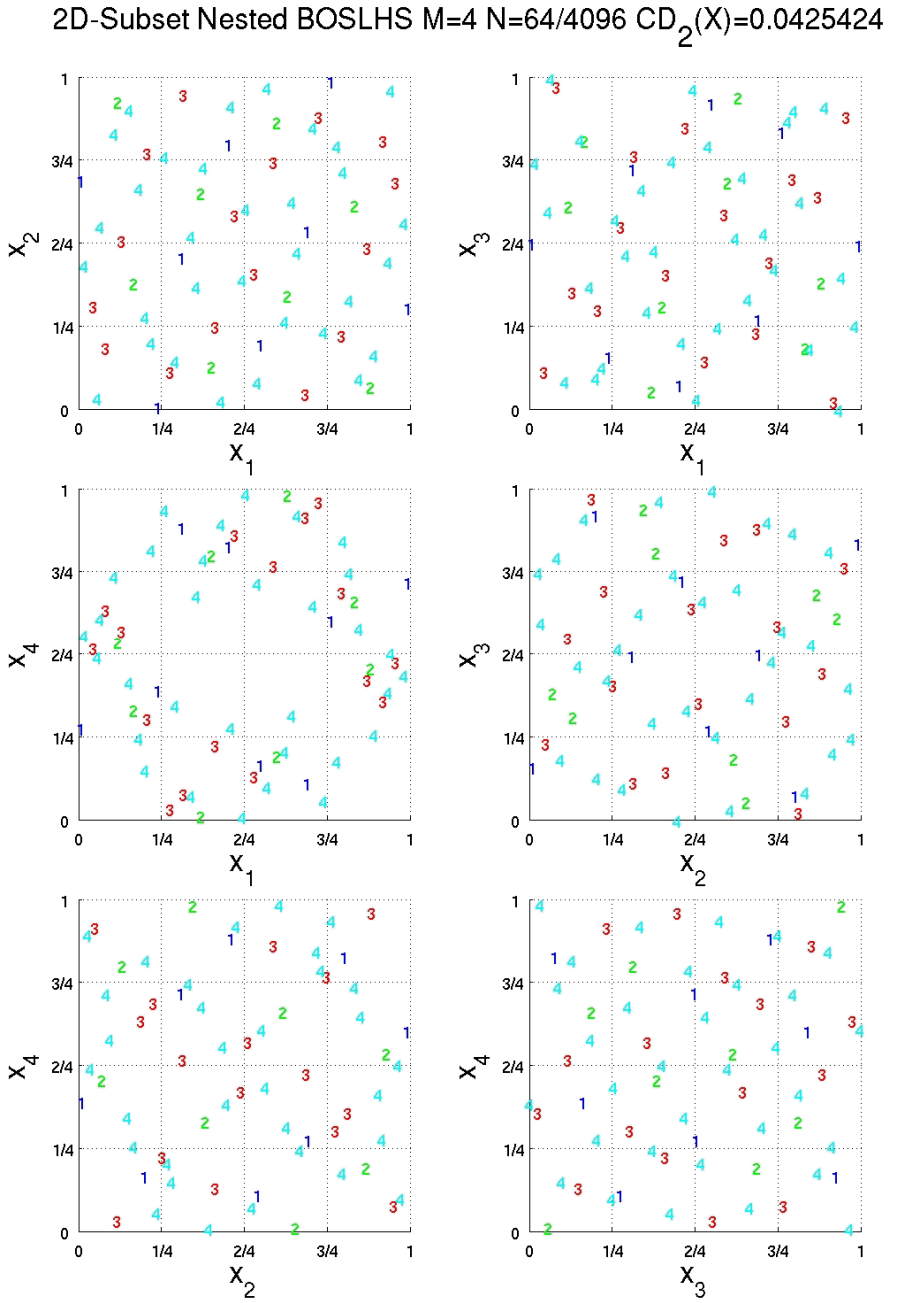
- BOSLHS has low discrepancy without being regular
- BOSLHS also scores well in other metrics: it has high "coverage," low correlations between dimensions, and a low (t,m,s)-net rating
- **VERY fast**: MATLAB generated a $N=2^{16}$ point M=8 dimensional space-filling **nested** BOSLHS design in ~8.21 seconds on an Intel 2.53 GHz processor (algorithms reported in literature take "minutes" for **non-nested** space-filling N = 100 point designs)
- By comparison, it took ~298.2 seconds ($O(N^2M)$ ops) to evaluate discrepancy for same design

Sample Design Quality Metrics
Other "partial" metrics

- **"Coverage"** (fraction of hypercube's volume filled by convex hull of points, VERY expensive for even moderately high dimensions)**: higher coverage is better**
- **Condition number of** sample design's **correlation matrix** (can be evaluated in $O(M^2N)$ ops)**: lower is better**
- **"t" quality metric** when design is considered to be a **tms-net** (quasi-Monte Carlo; metric moderately expensive $O({}_{(m-t+1+s)}C_s\ s\ b^m)$ ops where $s=M$, $b^m=N$)**: lower "t" is better**
- **NEW!** ***degree*** **of Binning Non-Optimality** (can be evaluated in $O(N \log(N))$ time)**: lower is better**

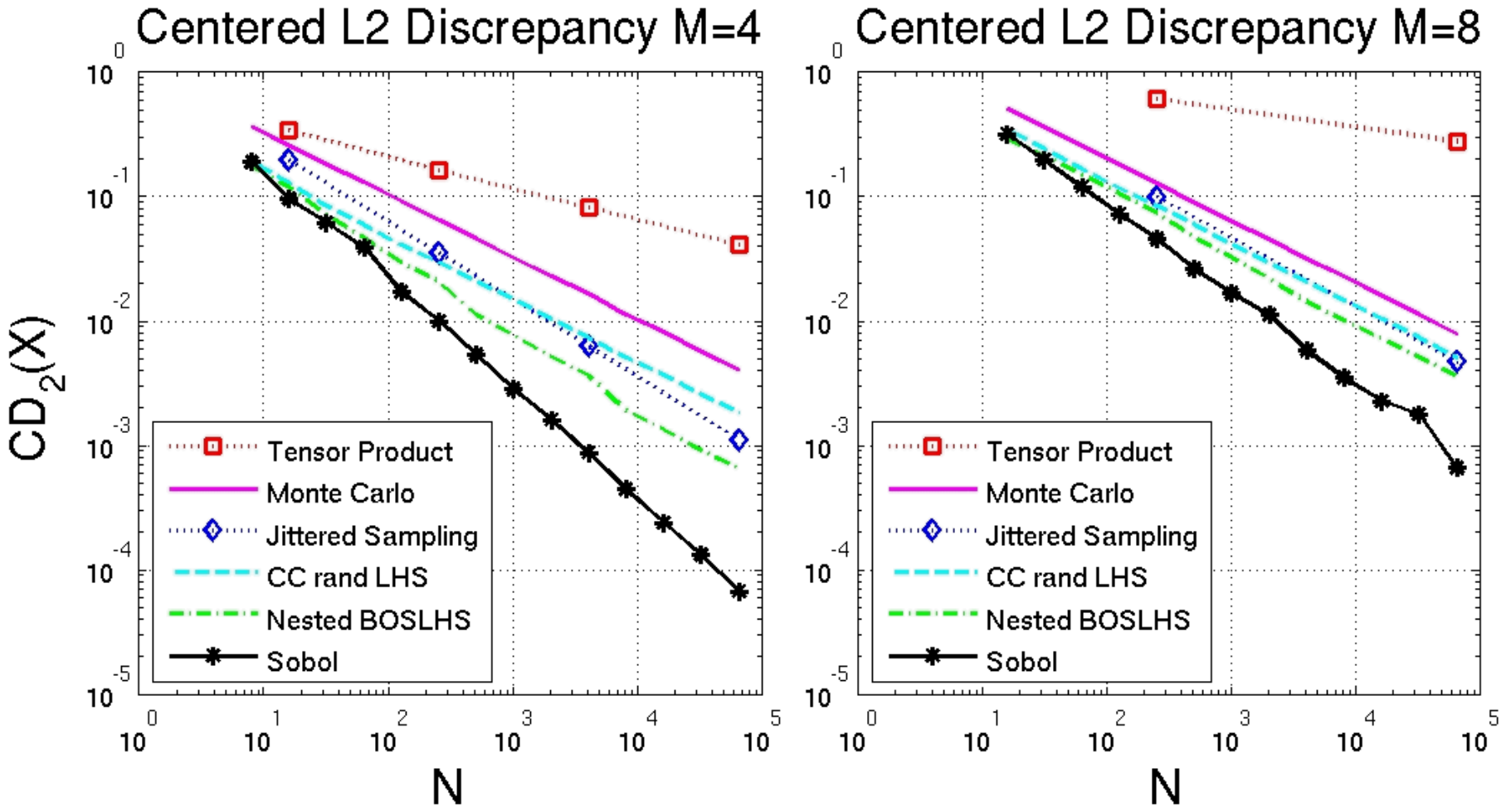
4-D Example

- Difference in 4 dimensions is in choosing maximally spaced bins
- In 2D, only 2^2=4 sub-bins per level, the 2*2=4 end points of 1 "orientation" (rotated set of orthogonal axes)
  - If 1 point in bin, new sub-bin is opposite old one
  - If 2 points (1 axis), 2 new sub-bins are other axis
  - Then go 1 bin deeper
- In 4D, 2^4=16 sub-bins per level, 2 orientations with 2*4=8 bins each
  - After first axis, randomly select order of other axes in same orientation
  - Then choose other orientation
  - Then go 1 bin deeper



Sandia National Laboratories

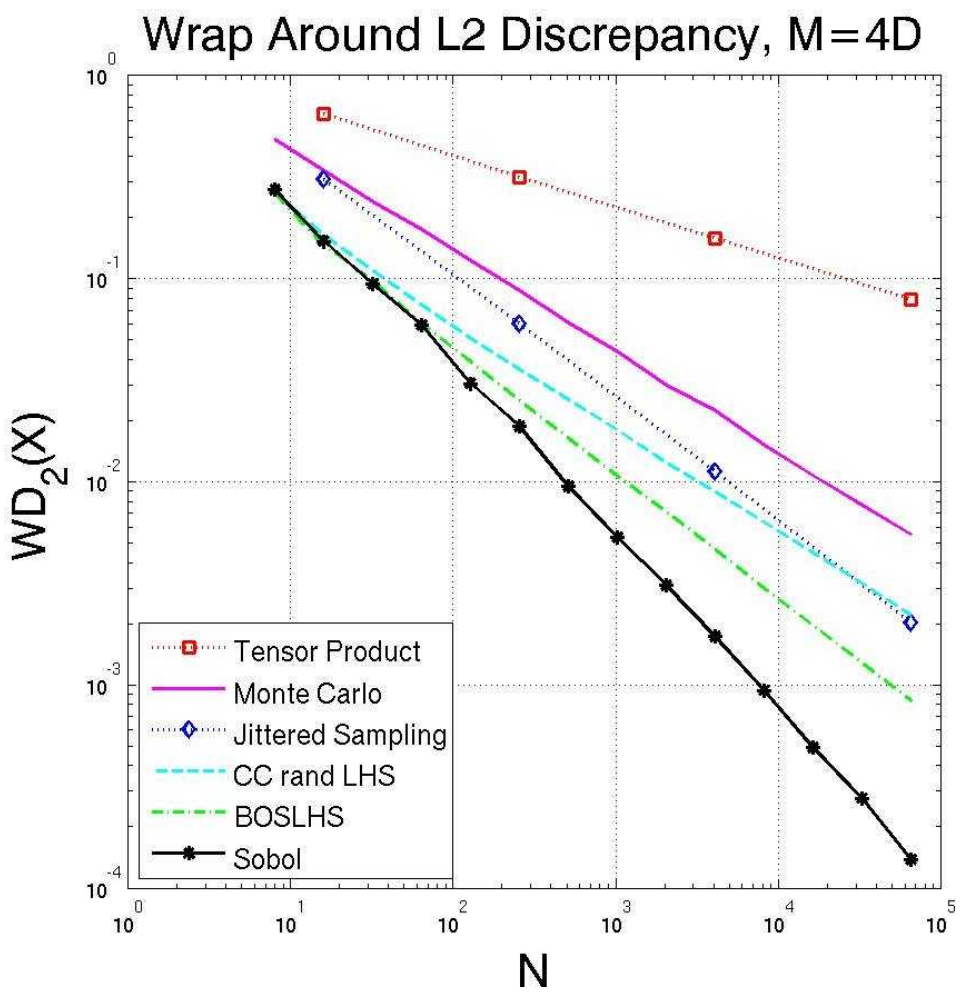
Results: Centered L2 Discrepancy (Lower is Better)

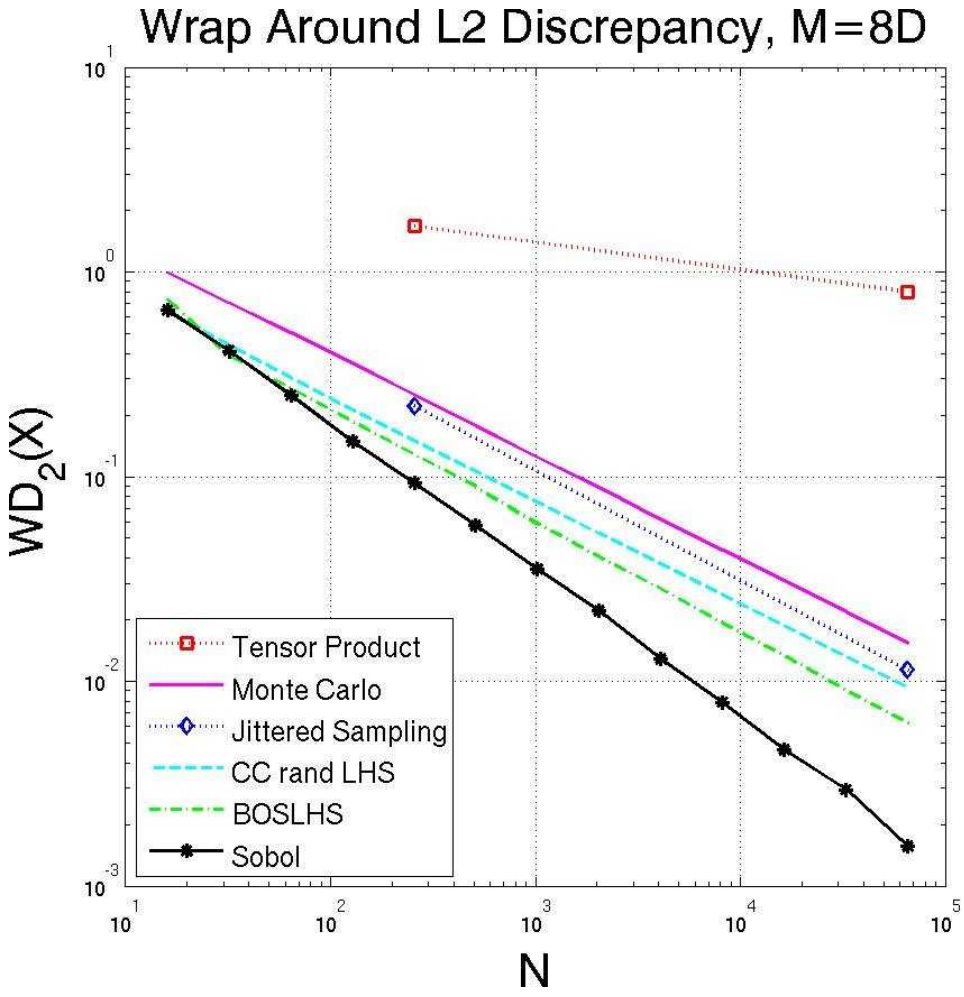


Plots are for average of 40 random designs

Sandia National Laboratories

Results: Wrap Around L2 Discrepancy (Lower is Better)

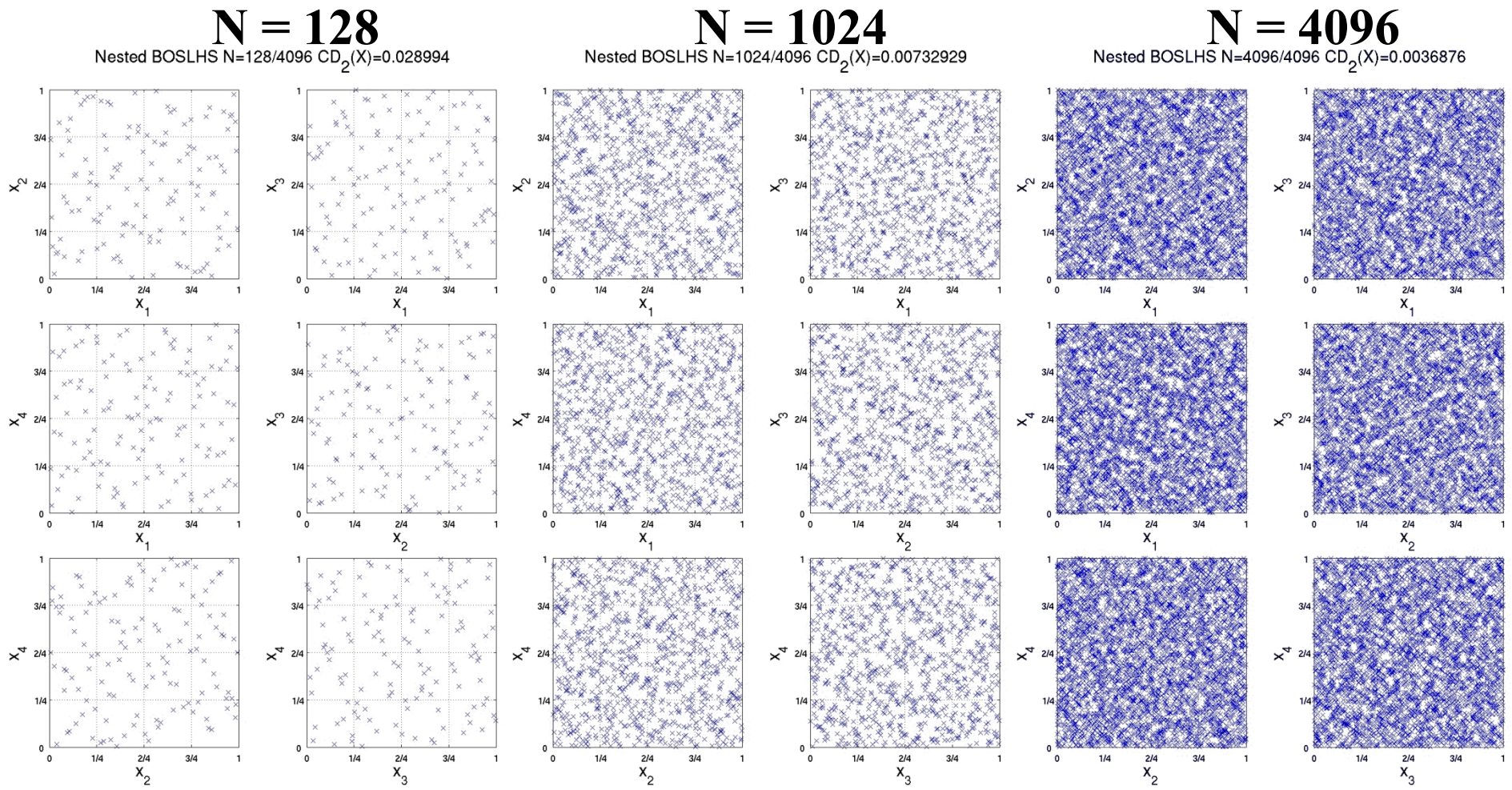




Plots are for average of 40 random designs

Sandia National Laboratories

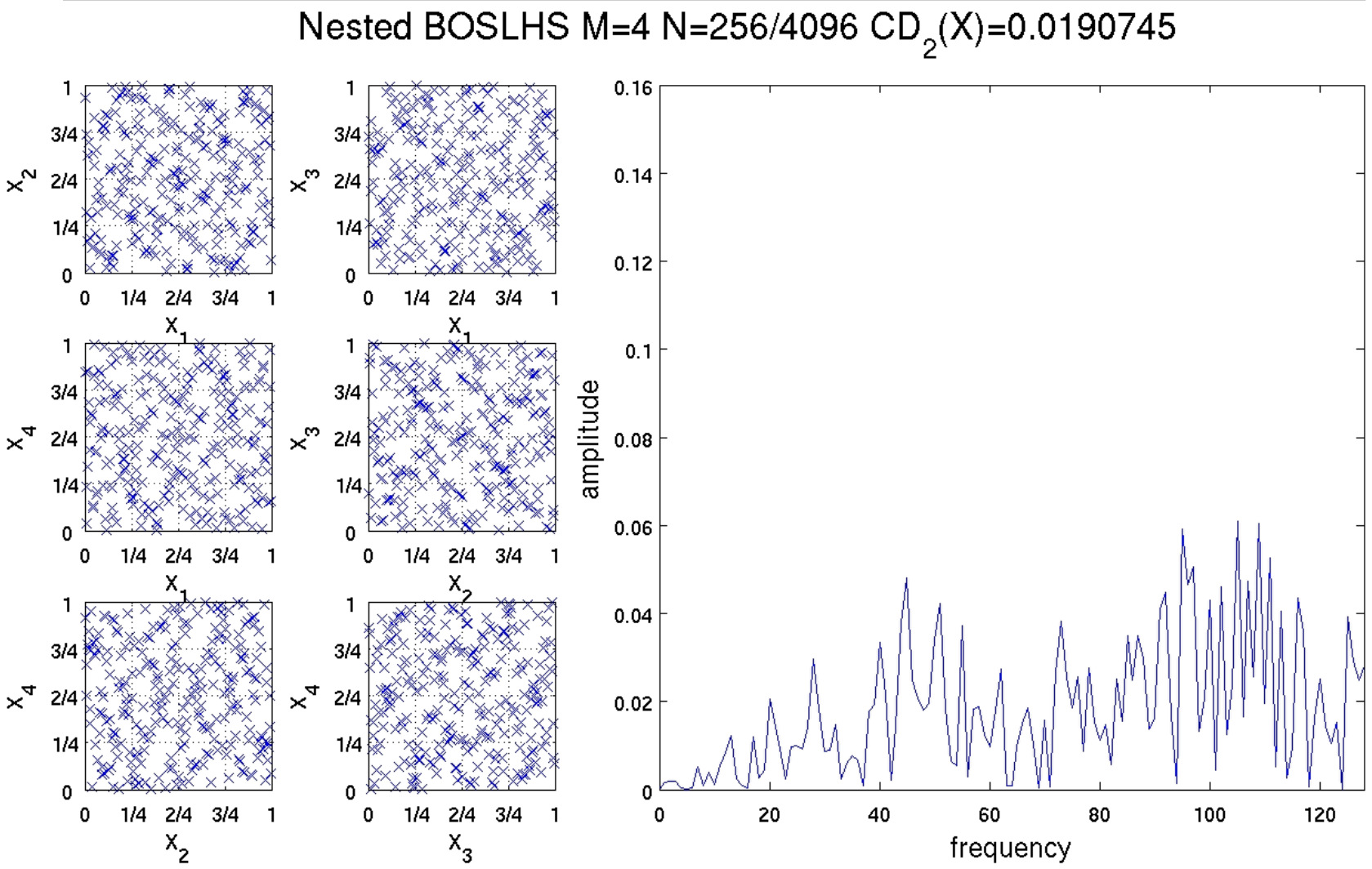
Results: Eyeball Metric M=4D



- Plotted all 6 combinations of 2 out of M=4 dimensions
- BOSLHS is visibly space-filling!

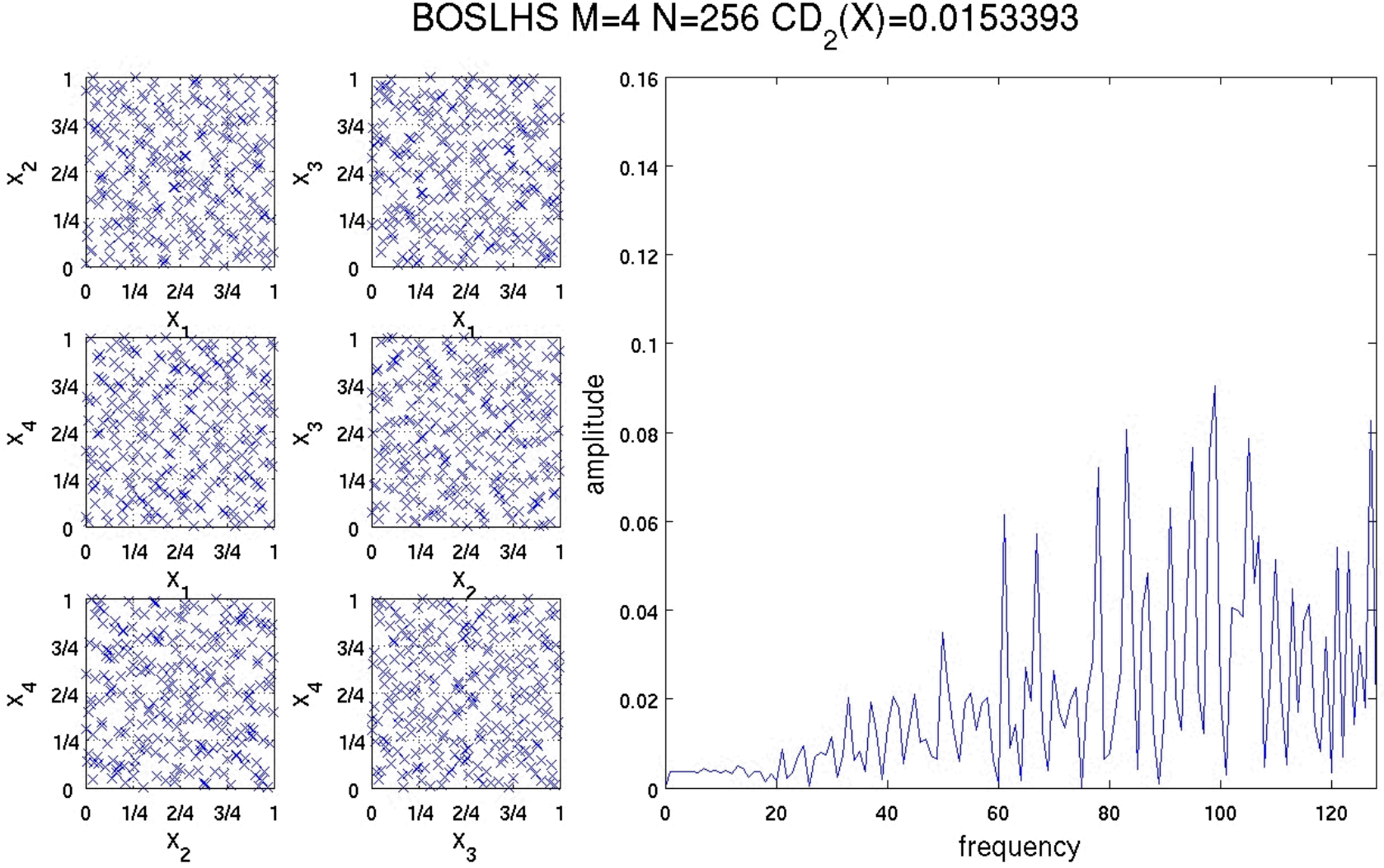
Sandia National Laboratories

Results: Nested BOSLHS Is Not Regular



Sandia National Laboratories

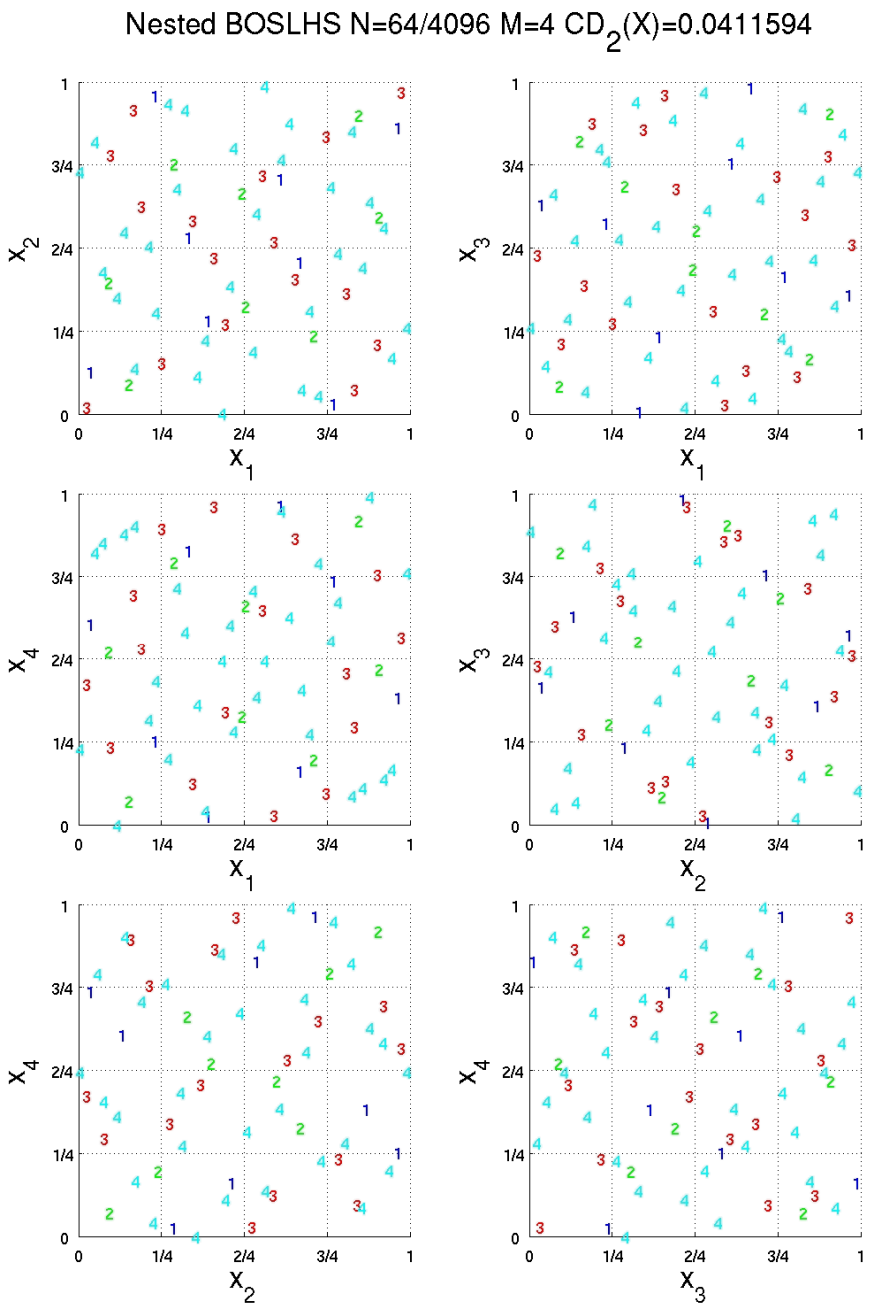
Compared To Original, Nested BOSLHS Less Regular But Higher Discrepancy



Sandia National Laboratories

4-D Example

- Difference in 4 dimensions is in choosing maximally spaced bins
- In 2D, only 2^2=4 sub-bins per level, the 2*2=4 end points of 1 "orientation" (rotated set of orthogonal axes)
  - If 1 point in bin, new sub-bin is opposite old one
  - If 2 points (1 axis), 2 new sub-bins are other axis
  - Then go 1 bin deeper
- In 4D, 2^4=16 sub-bins per level, 2 orientations with 2*4=8 bins each
  - After first axis, randomly select order of other axes in same orientation
  - Then choose other orientation
  - Then go 1 bin deeper



Sandia National Laboratories

Results: Coverage (higher is better)

"Coverage" for $M = 4$ Dimensions: Average of 40 runs

N	Binning Optimal Symmetric LHS	Cell Centered Random LHS	Monte Carlo Sampling	Jittered Sampling	Tensor Product Sampling
8	0.0717773	0.027062	0.0178996		
16	0.135135	0.104126	0.0916156	0.128427	0.0625
32	0.285717	0.233105	0.219465		
64	0.417035	0.372359	0.361626		
128	0.56022	0.522201	0.511982		
256	0.678416	0.647304	0.645049	0.667668	0.316406
512	0.773748	0.754804	0.749725		
1024	0.843177	0.832896	0.831007		
2048	0.896093	0.890245	0.886593		
4096	0.932229	0.928693	0.927748	0.929509	0.586182
8192	0.956723	0.954248	0.953466		
16384	0.97319	0.97129	0.971217		
32768	0.983415	0.982499	0.982312		
65536	0.989815	0.989387	0.98926	0.98965	0.772476

Results: Condition # of Correlation Matrix (lower is better)

Condition Number of the Correlation Matrix for $M = 4$ Dimensions: Average of 40 runs

N	Binning Optimal Symmetric LHS	Cell Centered Random LHS	Monte Carlo Sampling	Jittered Sampling	Tensor Product Sampling
8	1	14.6273	8.23719		
16	3.2505	4.14988	3.75258	2.39394	1
32	1.49974	2.27709	2.15406		
64	1.37672	1.76306	1.82367		
128	1.2064	1.4508	1.49656		
256	1.11022	1.32572	1.33407	1.10916	1
512	1.05589	1.21341	1.2108		
1024	1.0368	1.1546	1.14725		
2048	1.02121	1.09974	1.09939		
4096	1.01246	1.07576	1.07075	1.01254	1
8192	1.00717	1.04643	1.04922		
16384	1.00403	1.03608	1.03365		
32768	1.0027	1.02297	1.02461		
65536	1.00166	1.01872	1.01742	1.00145	1

Results: (t,m,s)-net, "t" quality metric (lower is better)

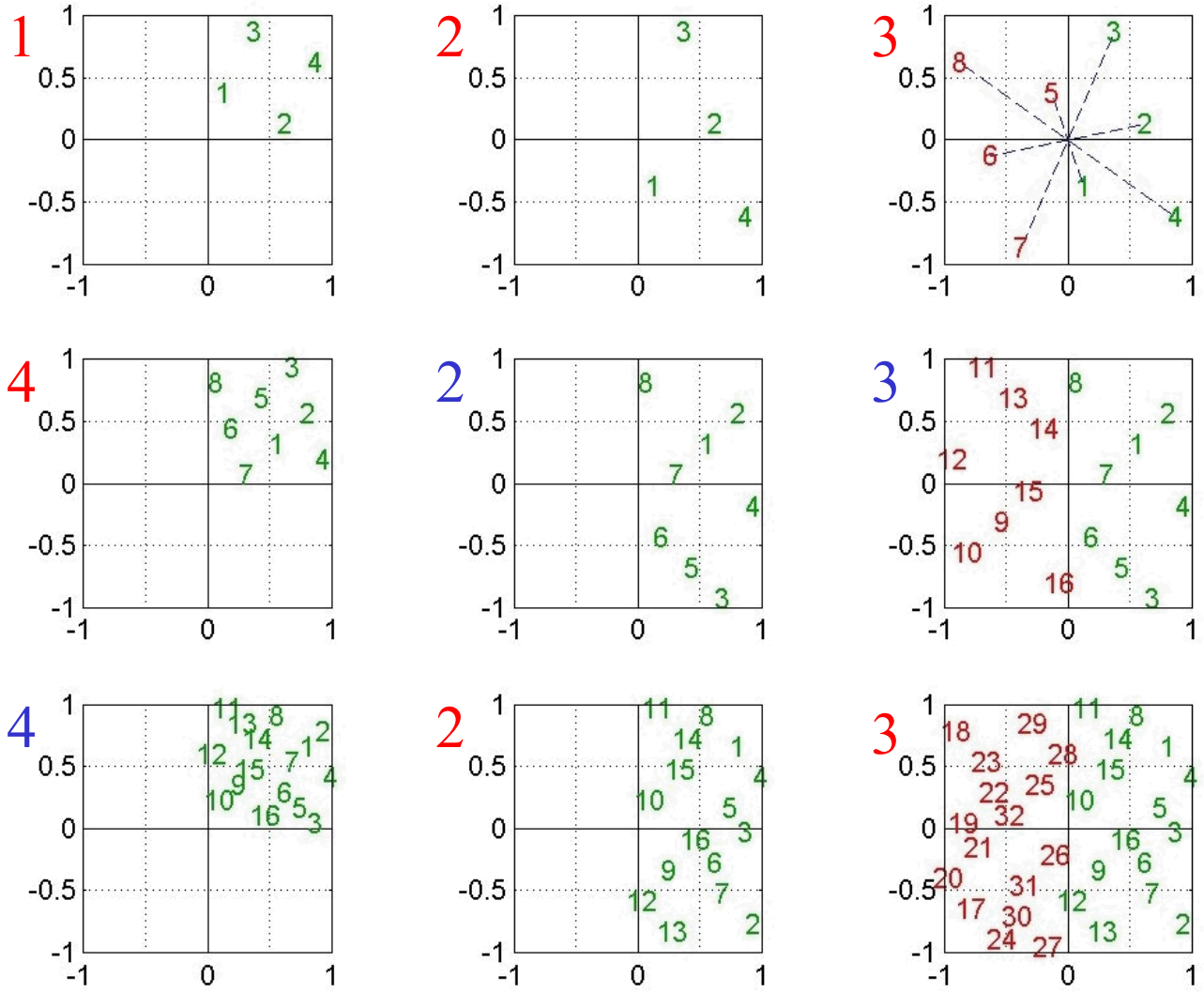
(t, m, s)-net Rating for $M = 4$ Dimensions: Average of 40 runs

N	Binning Optimal Symmetric LHS	Cell Centered Random LHS	Monte Carlo Sampling	Jittered Sampling	Tensor Product Sampling
8	(1 , 3 , 4)	(2 , 3 , 4)	(3 , 3 , 4)		
16	(2 , 4 , 4)	(3 , 4 , 4)	(4 , 4 , 4)	(3 , 4 , 4)	(3 , 4 , 4)
32	(2 , 5 , 4)	(4 , 5 , 4)	(5 , 5 , 4)		
64	(3 , 6 , 4)	(5 , 6 , 4)	(6 , 6 , 4)		
128	(4 , 7 , 4)	(6 , 7 , 4)	(7 , 7 , 4)		
256	(5 , 8 , 4)	(7 , 8 , 4)	(8 , 8 , 4)	(6 , 8 , 4)	(6 , 8 , 4)
512	(5 , 9 , 4)	(8 , 9 , 4)	(9 , 9 , 4)		
1024	(6 , 10 , 4)	(9 , 10 , 4)	(10 , 10 , 4)		
2048	(7 , 11 , 4)	(10 , 11 , 4)	(11 , 11 , 4)		
4096	(8 , 12 , 4)	(11 , 12 , 4)	(12 , 12 , 4)	(9 , 12 , 4)	(9 , 12 , 4)
8192	(8 , 13 , 4)	(12 , 13 , 4)	(13 , 13 , 4)		
16384	(9 , 14 , 4)	(13 , 14 , 4)	(14 , 14 , 4)		
32768	(10 , 15 , 4)	(14 , 15 , 4)	(15 , 15 , 4)		
65536	(11 , 16 , 4)	(15 , 16 , 4)	(16 , 16 , 4)	(12 , 16 , 4)	(12 , 16 , 4)

O(N log(N)) BOSLHS Algorithm

1. Start with n = 2M points that are well distributed in $(0, 1)^M$.
2. Select n/2 of the coordinates in each dimension other than the first to negate in such a way as to obtain n points that are well distributed in $(0, 1) \otimes (-1, 1)^{M-1}$.
3. Reflect the current n points through the origin to create n additional mirror points; this ensures that the design is symmetric.
4. Translate the 2n points from $(-1, 1)^M$ to $(0, 2)^M$, scale them to $(0, 1)^M$, and then set n = 2n.
5. Repeat steps 2 through 4 until the desired number of points has been obtained, i.e. until n = N.

O(N log(N)) BOSLHS Algorithm



Sandia National Laboratories

O(N log(N)) BOSLHS Algorithm

The tough part is step 2

Select n/2 of the coordinates in each dimension other than the first to negate in such a way as to obtain n points that are well distributed in $(0, 1) \otimes (-1, 1)^{M-1}$.

The easy (fast) answer is to recast the problem...

- Don't try change signs of dimensions individually
- **Send nearby points to octants that are far apart**

The Z-order quicksort will put nearby points in sequential order in O(N log(N)) ops

We just need a listing of octants in maximally spaced order