Space-filling experimental designs using sequences of lattices

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Outline

- Computer experiments and designs
- Applications
- New type of lattice design
- Nested structure
- Application in predictive science
- Re-cap

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Many processes are investigated using computational models

- Many scientific applications use **deterministic** mathematical models to describe physical systems

- To understand how inputs to the computer code impact the system, scientists adjust the inputs to computer simulators and observe the response

- The computer models frequently:
  1. require solutions to PDEs or use finite element analyses
  2. have high dimensional inputs
  3. have outputs which are complex functions of the inputs
  4. require a large amounts of computing time
  5. have features from some of the above

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Use Gaussian processes (GP's) for emulating computer model output

- GP' s have proven effective for emulating computer model output (Sacks et al., 1989; **Jones, Schonlau and Welch, 1998**) and also data mining

- Emulating computer model output
  - output varies smoothly with input changes
  - output is essentially noise free
  - passes through the observed response
  - GP' s outperform other modeling approaches in this arena

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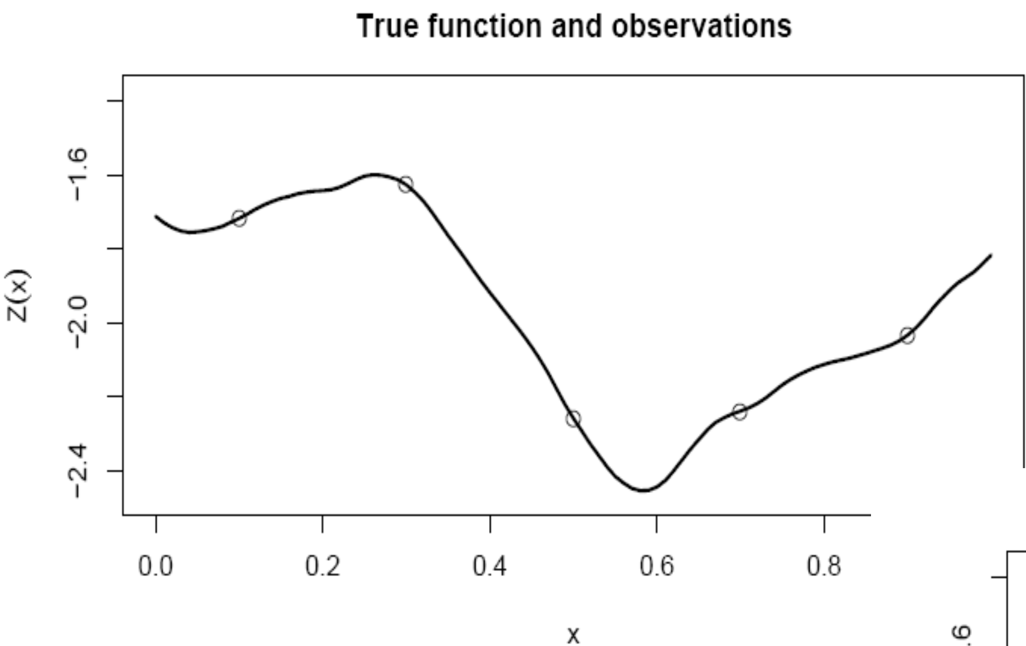
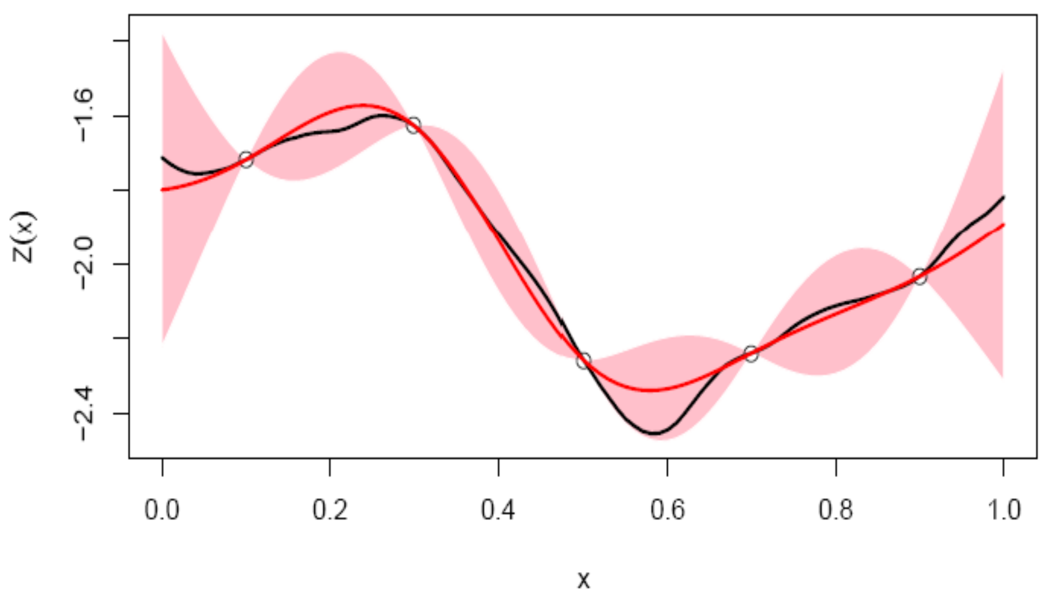
Why use a GP for emulation?



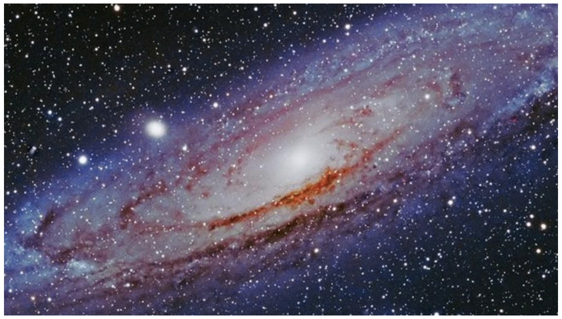
$$y(x) = \mu + z(x)$$

$$E(z(x)) = 0; \quad \mathrm{var}(z(x)) = \sigma^2$$

$$\mathrm{cov}(z(x), z(x')) = \sigma^2 R(x, x')$$

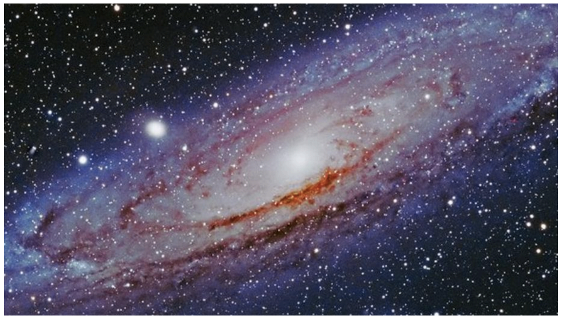


Applications of interest



- Upcoming space based cosmology missions promise exquisite measurements of the large-scale structure distribution of the Universe (e.g., including weak lensing, baryon acoustic oscillations, clusters of galaxies, and redshift space distortions)

- Currently exploring an 8-dimensional input space that, when combined with observations, should shed light into the initial conditions of the Universe and also the nature of dark energy



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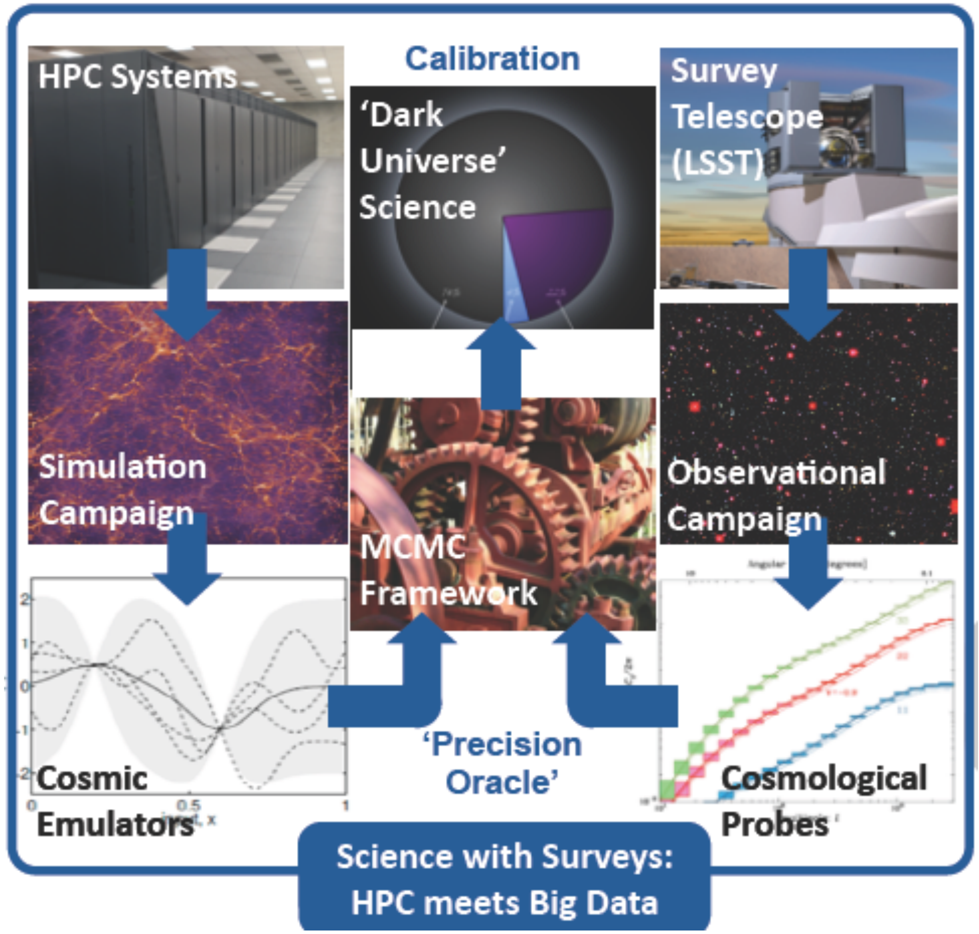

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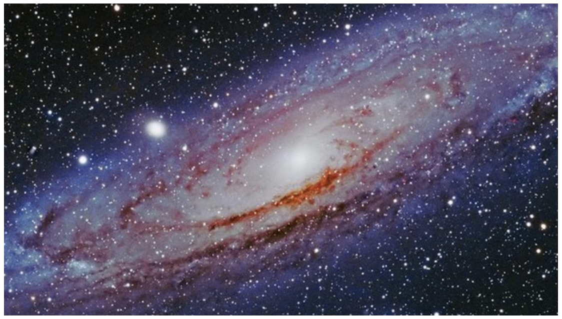

- Will be running about 100 simulations that should take between 1 and 2 years to complete … can run several of these in sequence
- Can investigate the response in intermediate stages while other simulations are running

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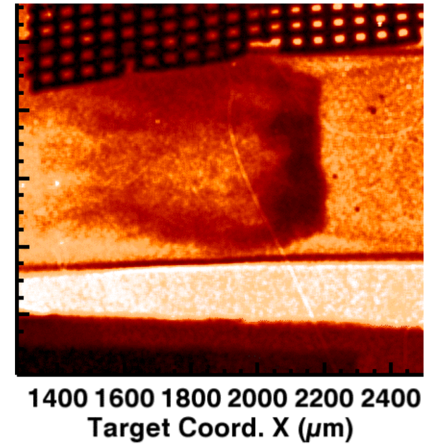


Applications of interest

- At the Center for Radiative Shock Hydrodynamics (CRASH), computational models were employed to simulate features of radiative shocks
- The CRASH codes consisted of high and low fidelity models
- It was helpful the run the high and low fidelity codes with the same inputs to explore the discrepancy between to two models
- The low fidelity code was run at far more input settings (high fidelity design was **nested** within the low fidelity design)

Design for computer experiments

- Johnson et al. (1990) and others (e.g., Kunsch et al., 2005) demonstrate that designs with good *space-filling* properties are essential for prediction using GPs
- Latin hypercube designs (McKay et al, 1989) and other variants (Tang, 1993) have proven popular
- For type of sequence of designs and low/high fidelity models, work by Qian (2009), Qian, Tang and Wu (2009) is related
- Designs based on Cartesian lattices have also been proposed (Beattie and Lin, 2004; Qian and Ai, 2010)
- Single state lattice designs have been discussed (Bates et al., 1996; **Pronzato and Müller, 2012**; He 2016, 2017)
- **Here, a new type of lattice design is proposed** (based on Heitmann, Bingham et al., 2016)

Would like our designs to have specific properties

1. Would like *n*-run designs where each design point is a *d*-dimensional input vector to the computer model

2. In our setting would like experiment designs (*D*) with good *d*-dimensional space-filling properties

3. Would like the designs to have the nesting property
   - Important for applications where good **intermediate-stage designs** are required, as well as the **final experiment design**

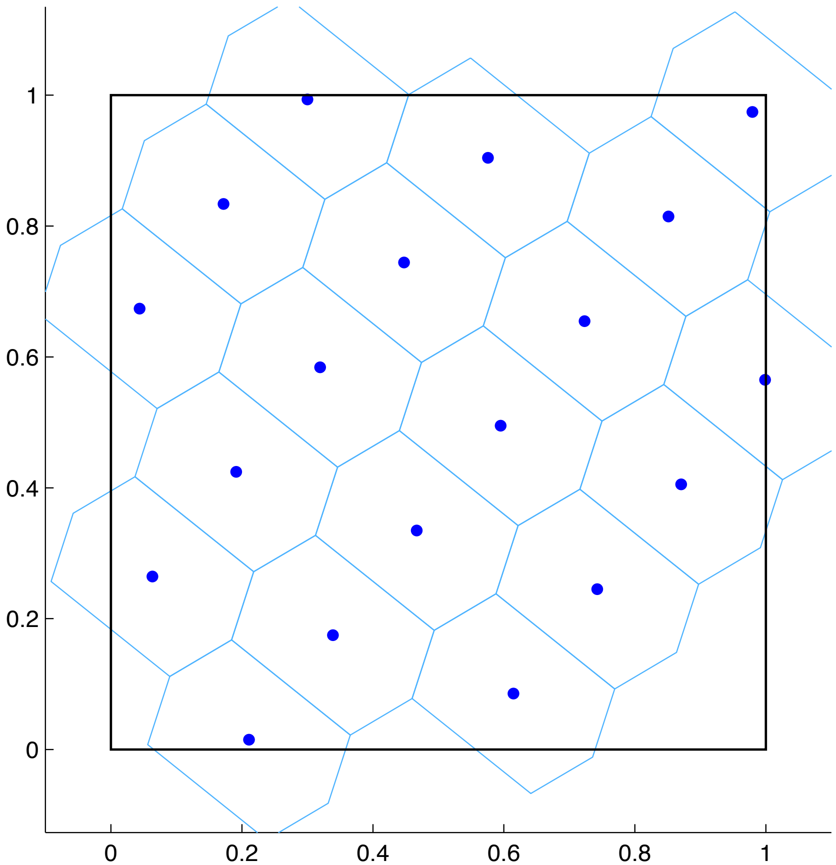
   - Important for applications with high- and low-fidelity simulators where the **high-fidelity simulator design is a sub-set of the larger, low-fidelity simulator design**

Suggestion …

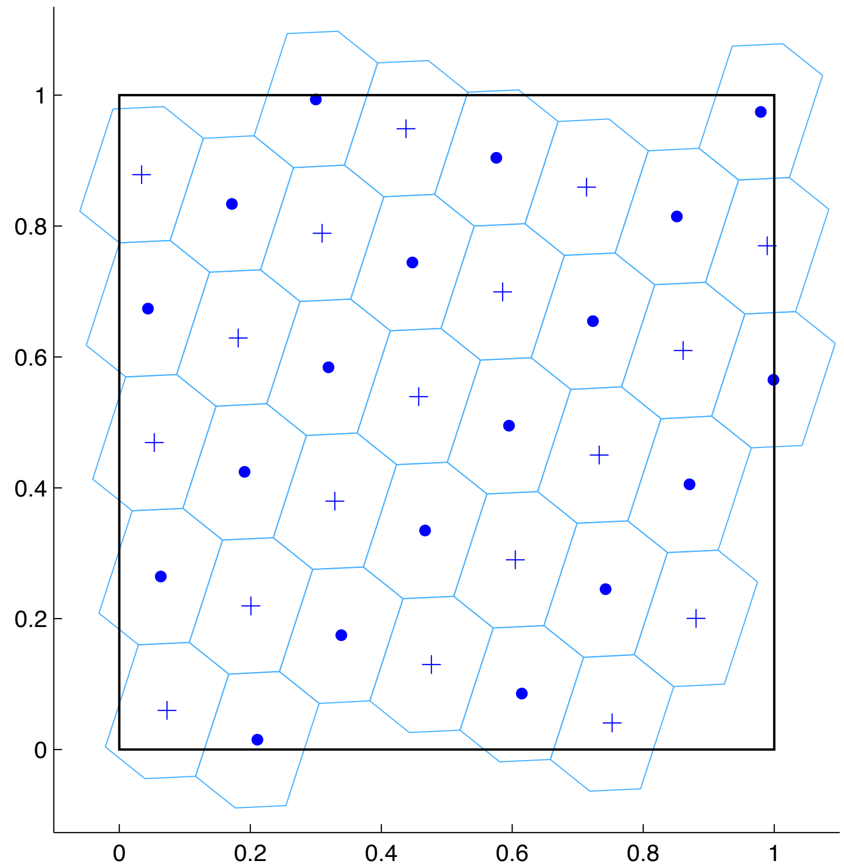
- Use a lattice
- For one-stage designs, can use already computed lattices (Conway and Sloane, 1999) that have good space filling properties
- Not quite as easy as you might think …
- Is more challenging for our setting where nesting is required

Example

First stage (high-fidelity) design



First and second stage (low-fidelity) design



Notation and definitions

- A **point lattice** is an infinite, discrete set of points in $\mathbb{R}^d$ that is constructed from integer multiples of a set of basis vectors in the columns of a *d* x *d* **generating matrix, G**,

$$\Lambda(\mathbf{G}) = \mathbf{G}\mathbb{Z}^d = \{\mathbf{Gk} : \mathbf{k} \in \mathbb{Z}^d\} \subset \mathbb{R}^d$$

- A **lattice design** $D(\Lambda, \mathcal{M}, \mathbf{p}) = \mathcal{M} \cap \{\Lambda + \mathbf{p}\}$ is the intersection of a point lattice and region $\mathcal{M} \subseteq \mathbb{R}^d$ that is shifted by a vector, $\mathbf{p}$

- See Conway and Sloane, 1999 or Patterson, 1954

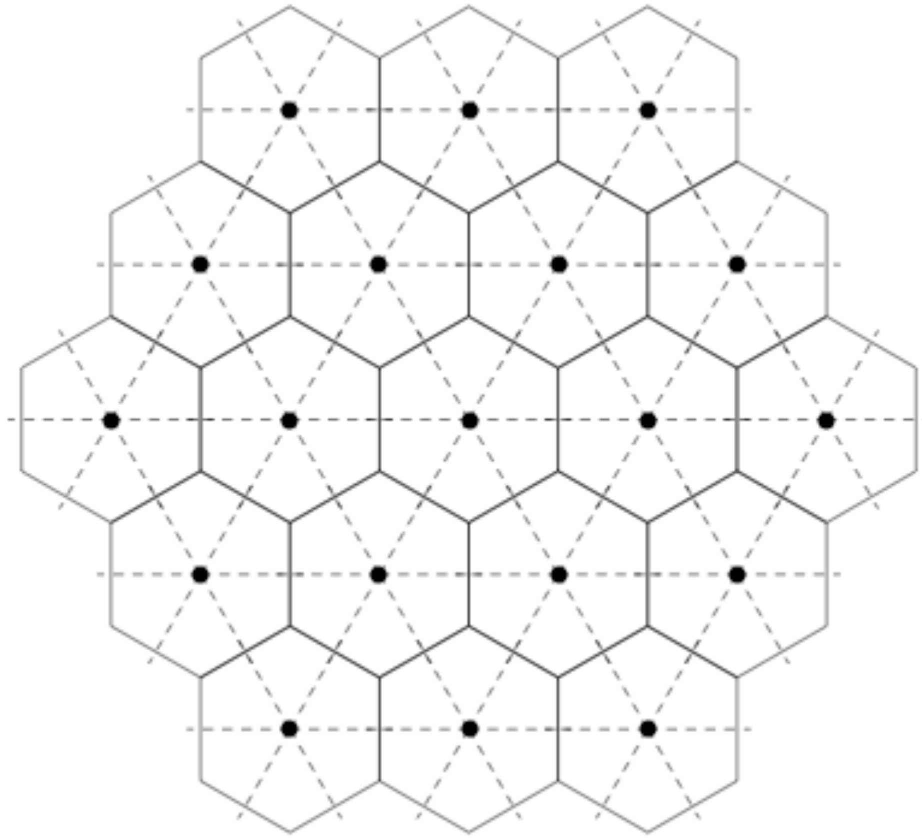
Usually the d-dimensional unit hypercube

Fun facts about lattices

- As a linear transformation of the integers, lattices inherit their abelian group structure
  - … this implies that the neighborhood around each lattice point is the same
  - This region is also called the **Vornoi cell**

- The space between the lattice points are described by the **fundamental parallelepiped**

Fun facts about lattices



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Example

- Factorial design (Cartesian lattice):

- Have d inputs with levels $\boldsymbol{s} = (s_1, s_2, \ldots, s_d)$

- Here $\mathbf{G}=\mathbf{I_d}$ and the lattice is $\Lambda(\mathbf{G}) = \mathbf{G}\mathbb{Z}^d = \{\mathbf{Gk} : \mathbf{k} \in \mathbb{Z}^d\} \subset \mathbb{R}^d$

- Region of interest is $[0,1)^d$ scaled by diag($\boldsymbol{s}$)

We are looking for specific designs

- A sequence of designs, is said to be nested if

$$D_l \subseteq D_{l+1} \text{ for all } l \in \mathbb{Z}$$

- Increasing l is called a **refinement** and decreasing l is called **coarsening**

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THE END

A result

- For two lattices, Λ_1 and Λ_2 , $\Lambda_1 \subseteq \Lambda_2$ iff there exists a matrix $\mathbf{K} \in \mathbb{Z}^{d \times d}$ that relates the generating matrices of the two lattices by $G_1 = G_2 K$. And under these conditions, if $|\det K| = 1$ then $\Lambda_1 = \Lambda_2$.

More notation and definitions

- A **dilation matrix,** $\mathbf{K} \in \mathbb{Z}^{d\times d}$, with $|\det \mathbf{K}| = \beta > 1$, applied to a lattice forms a nested sequence of lattices, $\Lambda_{l-1} \subset \Lambda_l$, via $\Lambda_{l-1} = \Lambda_l \mathbf{K}$

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- For this setting, an **admissible dilation matrix** is one where
  (a) $\mathbf{K}$ is a dilation matrix;
  (b) magnitude of all eigen-values of $\mathbf{K}$ are larger than 1; and
  (c) det $\mathbf{K} = \alpha^d$, where α is the eignen-value for $\mathbf{K}$

Theoretical results we can prove

- In $[0,1)^d$, the expected number of lattice points is $1/\det \mathbf{G}$
- $\mathbf{K}$ must be an integer matrix
- For refinement (i.e., l goes up) the volume of the fundamental parallelepiped decreases by $|\det \mathbf{K}| = \beta$
- Can show that to get a nested lattice $\beta > 1$, thus best refinement is to half the volume between points as the run-size is doubled

Why do all this fancy stuff?

- Dyadic sub-sampling is impossible for Cartesian lattices with $d > 2$
- For Cartesian lattices, number of lattice points grows exponentially with dimension
- **The main idea is to:**
  - use more general, non-diagonal generators, **G**
  - allow for sub-sampling rates that are 2, 3, 5, … (2 is most useful)

Why do all this fancy stuff?

- **Benefits**:
  - Sometimes can use general bases for known best packing or covering lattices, leading to a direct construction of maxi-min or mini-max designs, respectively
  - can consider virtually any run size
  - allows a sequence of designs that can be used in practical applications
  - Once bases are computed, do not need to recompute

How do we find designs

- Assume that the design region is $[0,1)^d$
- n is the experiment run size
- looking for a non-singular lattice generating matrix G that, when sub-sampled by a dilation matrix K with reduction rate $\beta = |\det K|$
- Need to find
  1. **G**
  2. **K**
  3. **Shift, rotation and scaling** to fit n points in the design region

How do we find designs

- Need some more theory:
- Restrict attention to designs where sub-sampled lattice is a scaled or rotated version of the original lattice
- **GK=QG**
- Preserves nice geometric properties… rotationally similar
- Imposes restrictions on **K**

How do we find designs… more theory

- The restriction (**GK=QG**) implies the choice of **G** up to rotation and scale … reason is that this implies that **K** and **Q** have same characteristic polynomial

- Can prove that: (i) for even d , there are 5 different **K**; and (ii) for odd d there is only 1 **K**

- Restricting to diagnolizable **K** and **Q**, finding **K** allows us to find **G** and **Q**

- We can still warp these **G** and we do so to optimize a desirable property (e.g., mini-max, maxi-min, correlation between columns of the design matrix)

- Finally, **G** is scaled so that $\mathbf{G}^*$=det c**G** = 1/n …

How do we find designs

- Finally, we can use the generating matric $\mathbf{G}^*$ and $\mathbf{K}$ to construct our lattice design

- However, the number of points in the region of interest is only expected to be n

- So, we randomly rotate $\mathbf{G}^*$ and also shift the lattice to achieve the desired run-size in $[0,1)^d$

Algorithms

Algorithm 1: Obtain a lattice with isotropic dilation matrix **K**

1. For given input dimension and sub-sampling rate construct isotropic dilation matrix **K**
2. Form the generating matrix, **G**

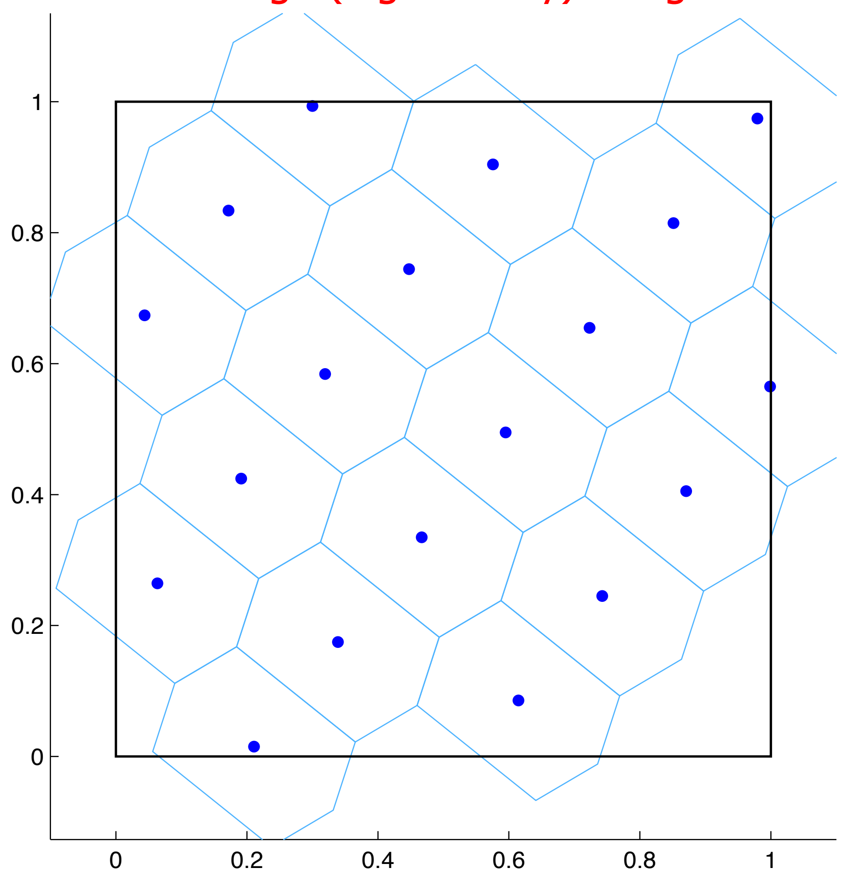
Algorithm 2: Produce a lattice design in the unit hypercube

1. Consists of finding possible designs under random shifts, **p**, of the lattice given **G**, **Q** and **K**
2. Effective to first determine points in a bounding box of design region and then find which of these points are in design region

Algorithm 3: Can further refine based on random shifts, **p**, and rotations $\mathbf{Q}^*$, to optimize additional properties

Example

First stage (high-fidelity) design



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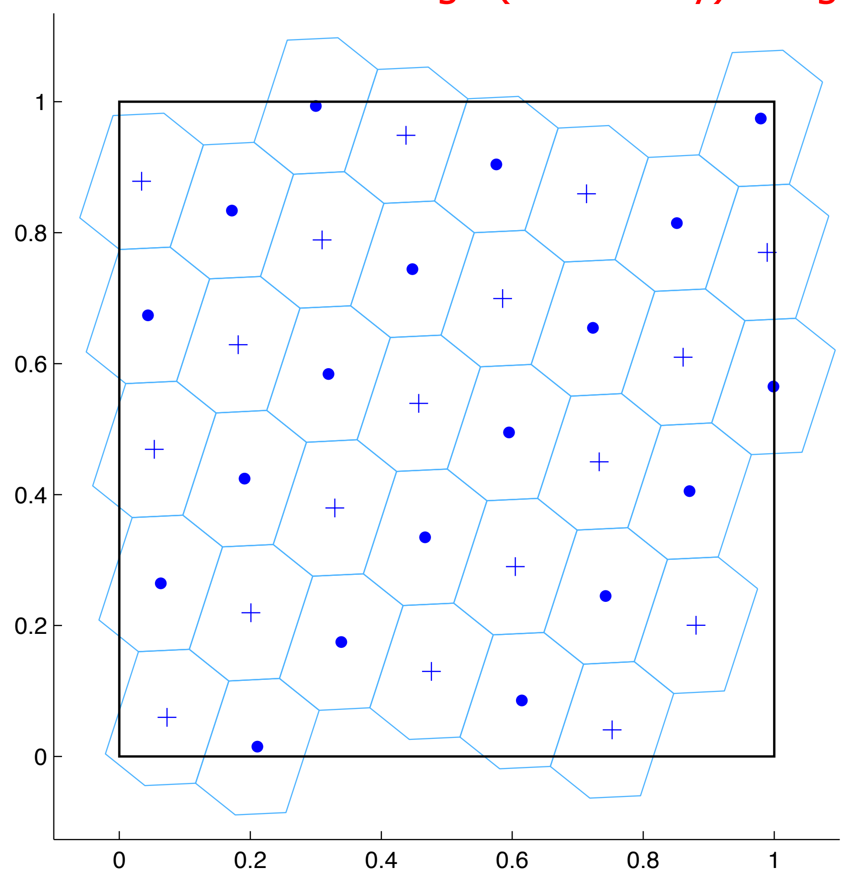
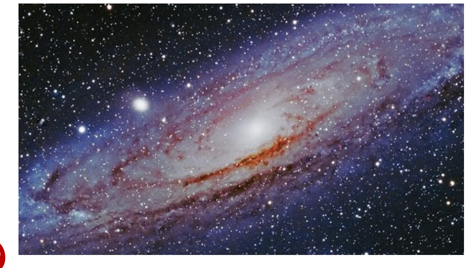
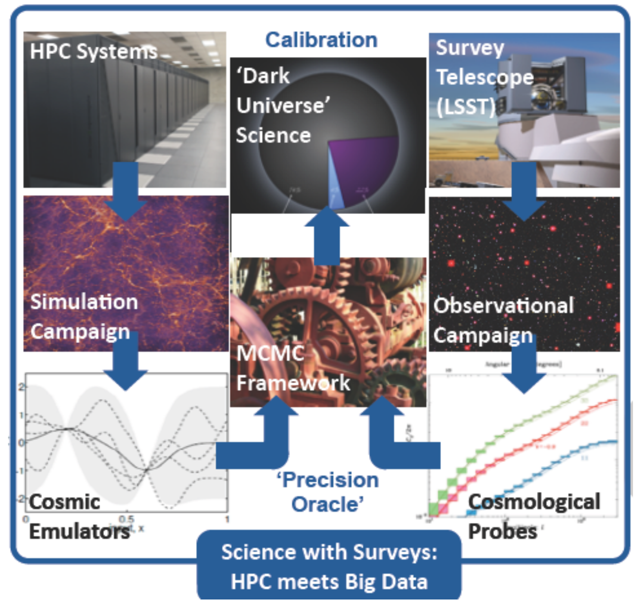




Cosmology – what did we do?

- Had 8-dimensional input space, n=100 runs in 3 stages:

$$
\begin{aligned}
0.12 \le\ & \omega_m \le 0.155 \\
0.0215 \le\ & \omega_b \le 0.0235 \\
0.7 \le\ & \sigma_8 \le 0.9 \\
0.55 \le\ & h \le 0.85 \\
0.85 \le\ & n_s \le 1.05 \\
-1.3 \le\ & w_0 \le -0.7 \\
-1.5 \le\ & w_a \le 1.15 \\
0.0 \le\ & \omega_\nu \le 0.01.
\end{aligned}
$$



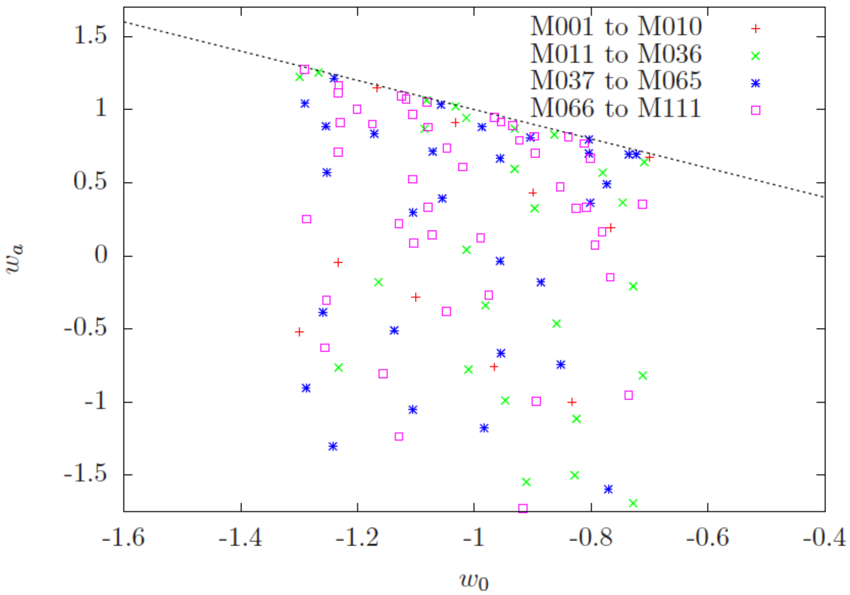
Cosmology – what did we do?

- Had a low-fidelity model (linear power spectrum) to test the efficacy of the designs

- Used a 3-stage lattice design n_1=25; n_2=25; n_3=50 (optimized via maximin criterion)
  - Ran each design on the low-fidelity code and did intermediate analyses (i.e., after 25 runs, 50 runs and finally 100 runs)
  - Turned out that several of the runs produced non-physical results
  - Had to do with implicit constrains on the dark energy parameters

Cosmology – what did we do?

- Instead, re-did the design procedure using the constraint $w_a + w_o < 0$



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Re-cap

1. Have proposed a new type of lattice design that is useful in a variety of applications

2. Can be used to find designs with good space filling properties

3. Can find large designs from small ones

4. We are pre-computing good bases for different *d*

Thank you for indulging me

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- Sub-sampling a lattice such that the chosen sample is **also a lattice** is performed by right-multiplying an integer dilation matrix onto G

- **Dyadic sub-sampling**: discards every second point in each basis vector direction (**K**=2**I**; $\beta = 2^d$)