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Hybrid Designs: Space Filling and Optimal Experimental Designs for Use in Studying Computer Simulation Models

Rachel Johnson Silvestrini PhD
Assistant Professor
Operations Research Department

Outline

- Computer Simulations
- Metamodeling
- Types of Experimental Designs
- A Hybrid Experimental Design Approach
- Example Using a ISR Simulation Model
- Questions

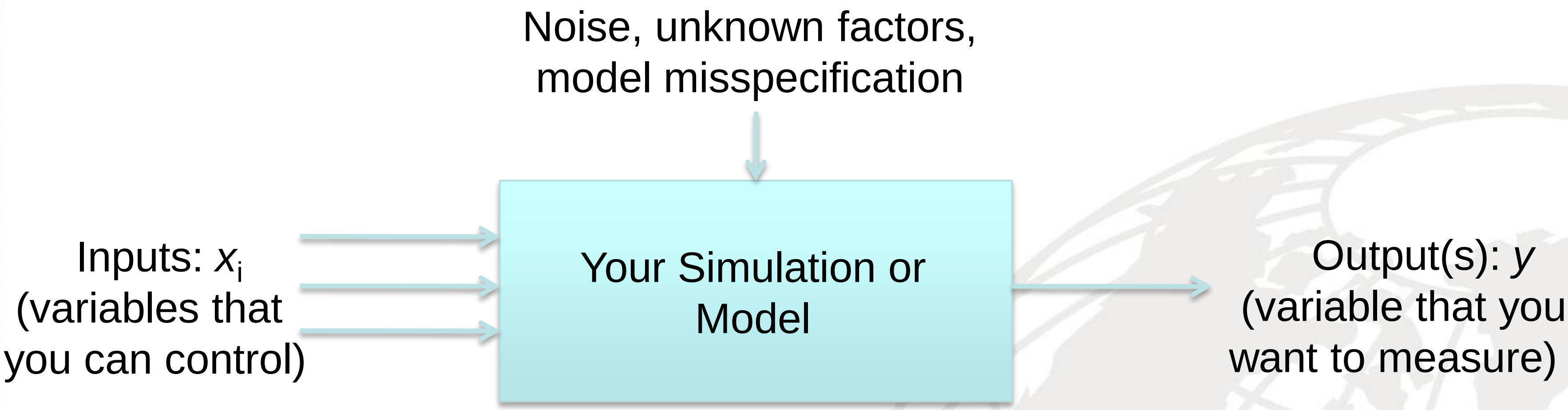
Computer Simulations

- Computer simulation models are built to mimic reality
- We ***do not*** always treat computer simulations like reality
  - Lots and lots of experiments are run
  - Many experiments are run that are prohibited in the real world
- We ***do*** often treat computer simulation results as if they were reality

Types of Simulation Models

- Stochastic
  - Output is a random variable
  - Blocking and randomization not an issue, but replication is
- Deterministic
  - For a given set of inputs, the output will be the same each time the model is run
  - Blocking, randomization, and replication are irrelevant

Illustration and Definitions



- Let's assume that there is some underlying model: $y = f(x) + \varepsilon$
- This model (often called a metamodel) can be:
    - mechanistic
    - empirical
        - linear regression model
        - non-linear model
        - generalized linear model
        - Gaussian process model (aka Kriging)
- A goal of *Experimental Design*: find/fit a metamodel

Simulation Needs

- People who run simulation models sometimes have trouble choosing what conditions to run (input levels to select) in order to fully characterize the input domain
- Additionally, once those conditions are selected, it might be difficult to describe the outputs in a meaningful way
- Experimental design and analysis provides a way to
  - Choose conditions to run your model (i.e. select inputs)
  - Find a suitable mathematical model that allows you to summarize your input-output data

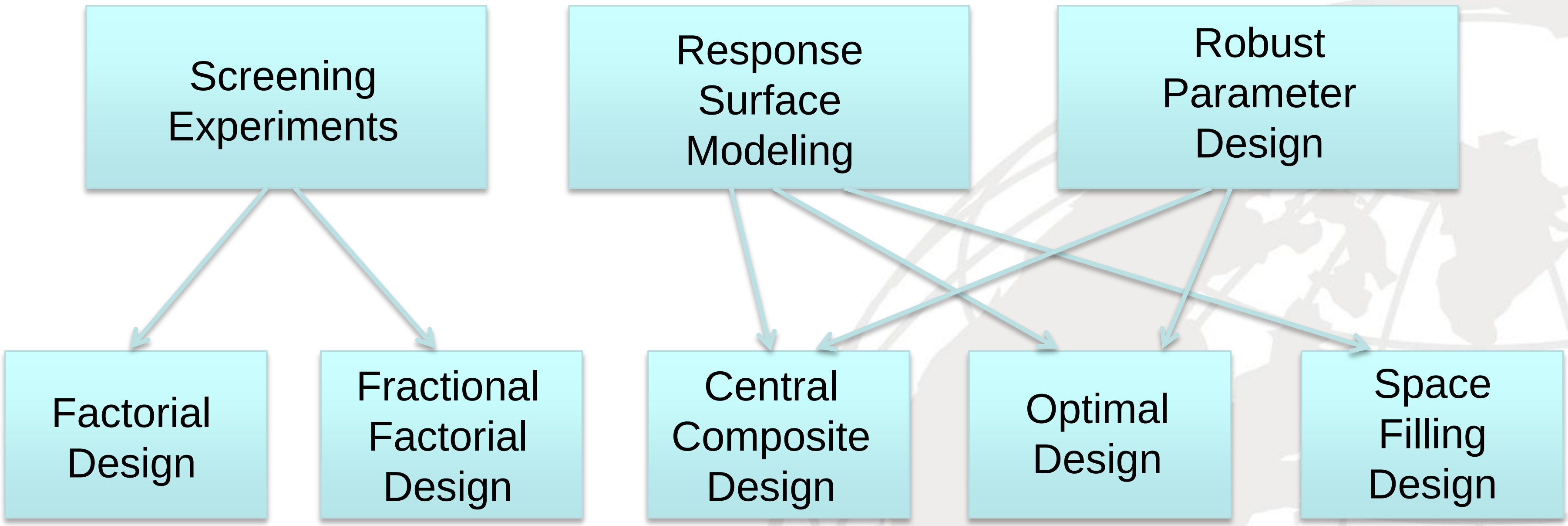
Metamodeling: What is it?

- After we run a computer simulation we would like to relate the inputs to the output(s) through the use of a closed form mathematical expression [1,4]
- Examples of common empirical metamodels used in practice:
  - Linear regression models (i.e. polynomial models) [1,4]
  - Non-linear models (i.e. logistic regression model) [8]
  - Gaussian Process models (i.e. Kriging) [4,9]

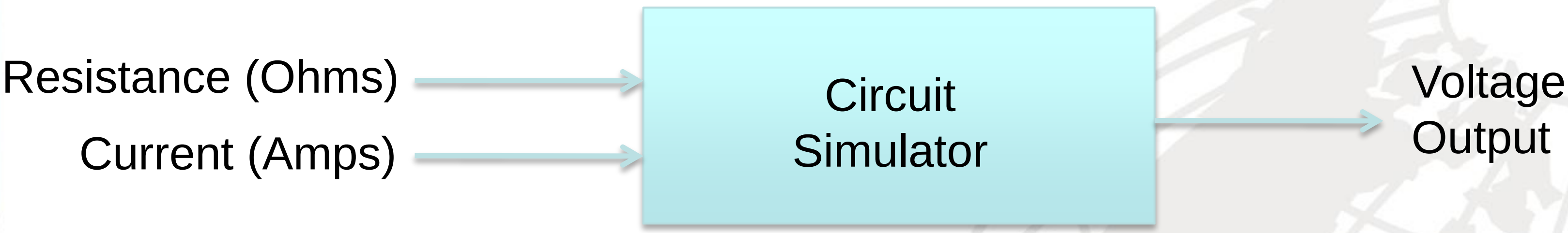
Experimental Designs

- The choice of experimental design can strongly influence how “good” your results are
- Can create most designs in standard software packages such as JMP or Design Expert
- Require you to list
  - Inputs (including input values or ranges)
  - Output(s)
  - Number of runs (trials you are willing to perform)
  - If running optimal design – must specify assumed model

Experimental Designs are Based on Goals

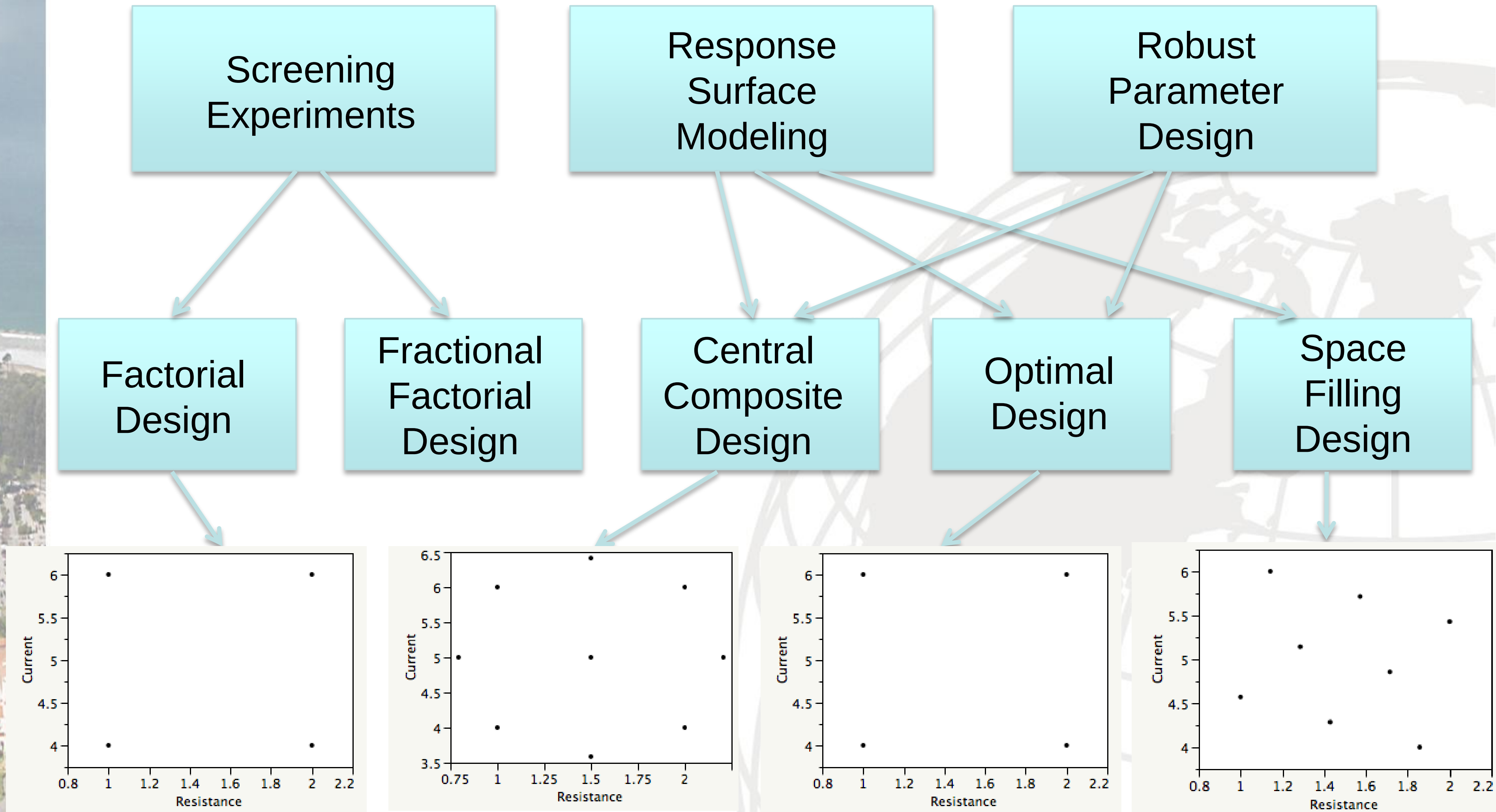


A Quick Example: Studying Ohm's Law



Input Factor	Range	Variable Type
Resistance (ohms)	[1 – 2]	Continuous
Current (amps)	[4 - 6]	Continuous

Experimental Designs are Based on Goals



Optimal Experimental Design

Optimal Design (examples: *D*-optimal and *I*-optimal)

- Pros
  - Great for creating empirical models of many forms (especially useful if using the linear regression approach)
  - Useful for constrained design spaces
  - Optimal designs for many linear regression models are the standard designs (i.e. 2^k)
- Cons
  - Requires specification of the metamodel before collecting any data
  - Non-linear optimal designs are dependent on unknown parameters

Space Filling Experimental Design

Space Filling Design (examples: Latin Hypercube and Uniform)

- Pros
  - Fill the design space
  - Useful for unknown metamodel choices
- Cons
  - Don't cover the corners of the design space

Experimental Design Approach

- What if you don't know *a priori* what type of metamodel will work best for your results?
- Is there some type of experimental design that can be used assuming you may choose several type of metamodels to use?
  - Yes
  - A hybrid design approach that combines optimal design with space filling design
    - Provides coverage to the corners of the design space and the interior
    - Useful for fitting linear regression models and for fitting metamodels you might not have planned for

Situations Useful for Hybrid Design

- Situation 1: You are running a simulation experiment and would like good coverage of the design space. You are not sure what metamodel you will use, but think that a linear regression model choice is among the possibilities

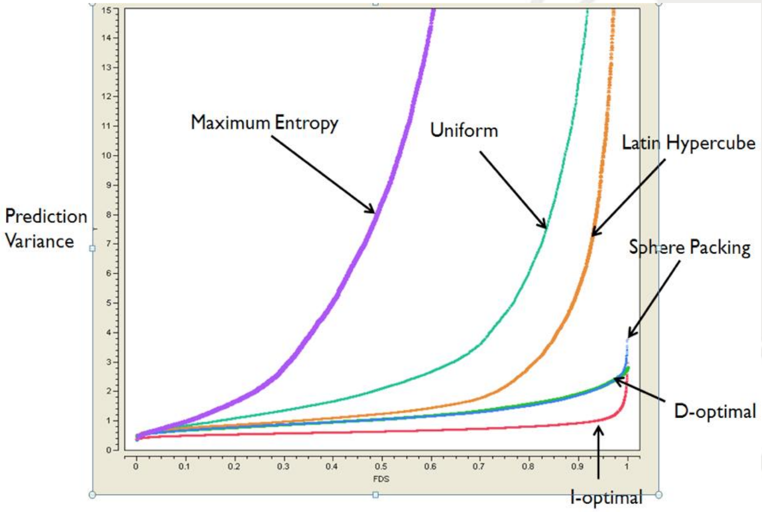
- Situation 2: You are running a simulation experiment and will most likely fit a linear regression model, but would like to simulation some "random" trials to use as either
  - Cross-validation or
  - If your model is making bad predictions, points that can be used to fit new models

Research Comparison Method

- Previous research on these designs compared optimal, space filling designs, and hybrid designs based on:
  - Scaled prediction variance
    - For the linear regression model: $\frac{N\,V[\hat{y}(x_o)]}{\sigma^2} = N\boldsymbol{x}_o'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x}_o$
    - For the Gaussian process mode:
  - Fraction of Design Space plots [11]: plot the empirical distribution function of scaled prediction variance over the design region
  - Used in the assessment of prediction capability [8]

Example FDS Plot

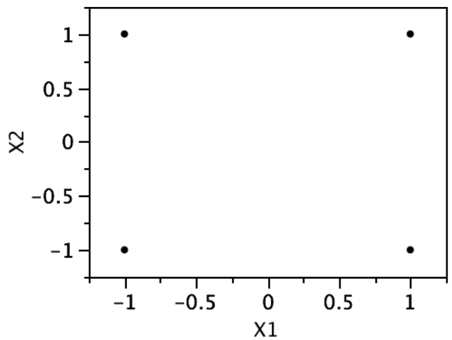
- Designs created for the case with
  - 2 input factors
  - 2nd order polynomial
  - Sample size = 10



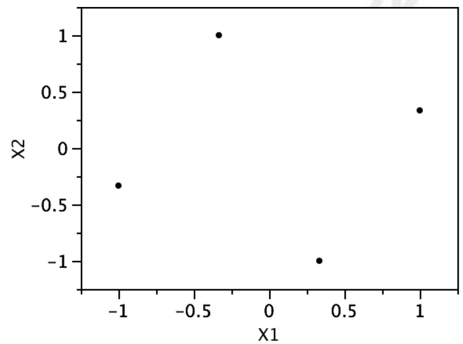
Hybrid Design Development

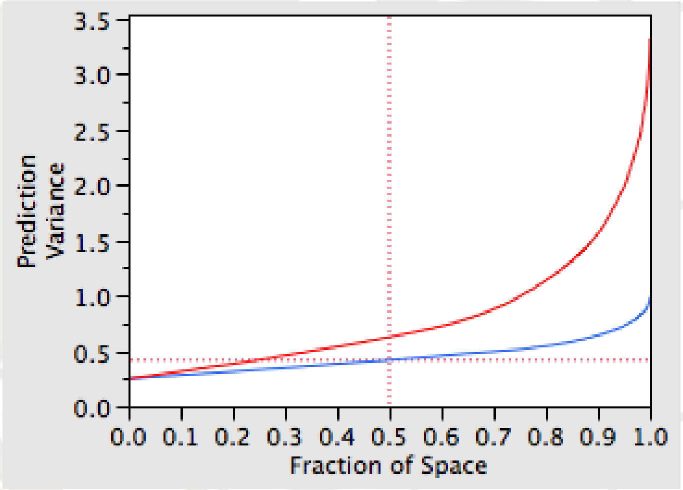
- Consider a saturated design for two factors and an anticipated main effects and two factor interaction model
- Here is an example of what the I-optimal design (a) and a Latin hypercube space-filling design (b) look like and their associated FDS plots

a) *I*-optimal



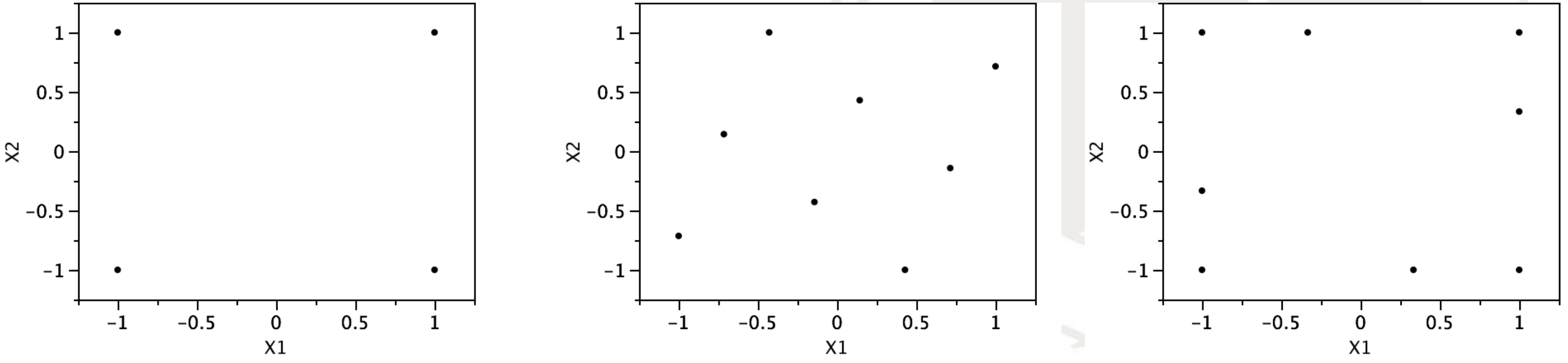
b) Latin hypercube



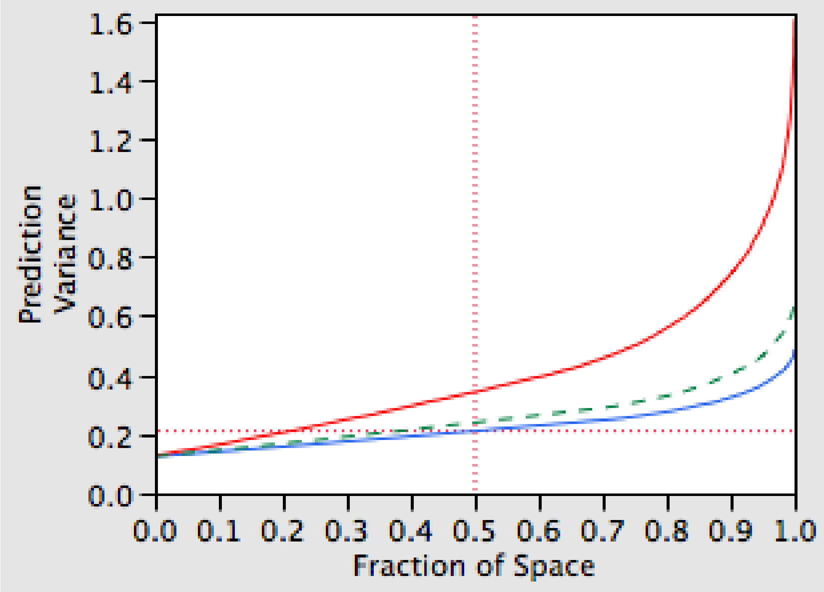


Hybrid Design Points

- We augmented the space-filling design with optimal points
- Why?
  - Wanted the space-filling design because it fills the interior region of the design space
  - Wanted the optimal design points



Performance of Hybrid Design

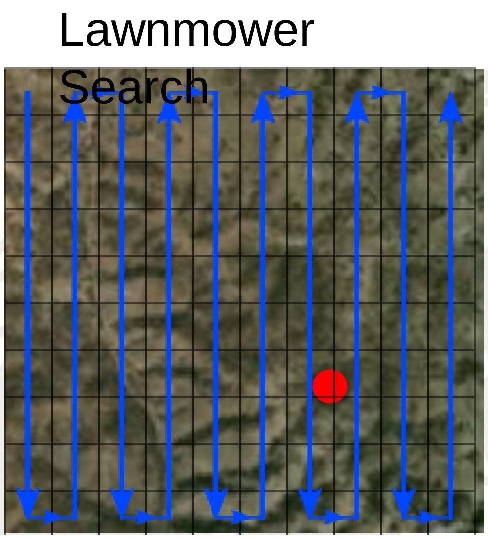


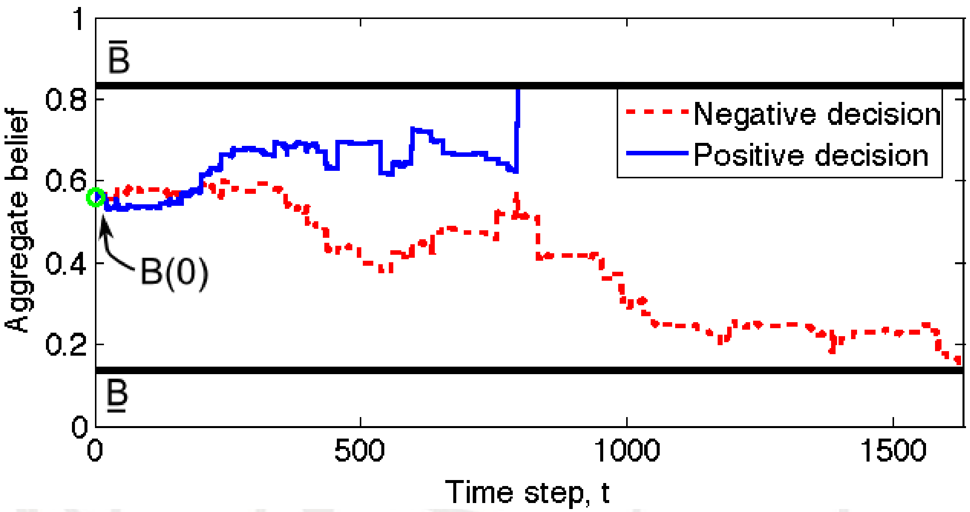
ISR Application

- Unmanned systems can play a prominent role in diverse information gathering missions such as:
  - Search and Rescue (SAR)
  - Intelligence, Surveillance and Reconnaissance (ISR)
- Current research on unmanned system search requires the use of sophisticated sensing, computation, coordination, and communication capabilities
- This example is based on research conducted by a colleague (Timothy H. Chung) and I
- The work presented seeks to revisit the used of exhaustive search strategies as the basis of the search process and leverage new probability models as well as experimental design to help inform and refine concepts of operations

The ISR Simulation

- Consider an area of interest with a missing person or a target
- A simulator was built to mimic an unmanned system searching the area
- The simulator updates probabilities about the location of the person as a function of time and observation
- The goal of the study is to study the effect of several inputs of interest on five response variables



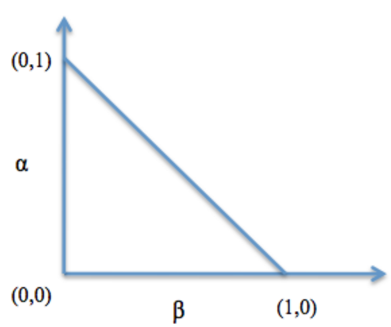


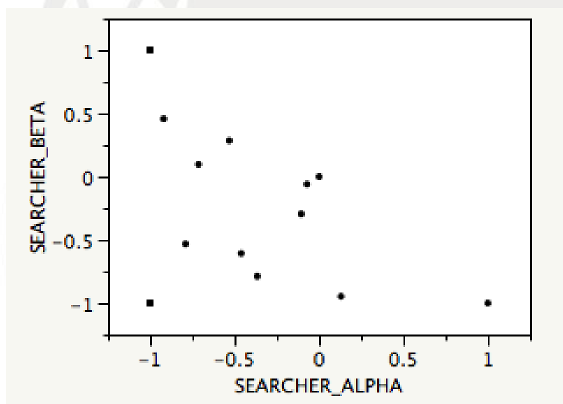
Hybrid Design Approach

- Combined D-optimal design points with uniform design points
- The inputs are:

Factor	Label	Description	Range or Levels
α	x_1	False positive detection error	[0.0, 1.0]
β	x_2	False negative detection error	[0.0, 1.0]
$B(0)$	x_3	Initial aggregate belief	[0.3, 0.7]
$\overline{B}$	x_4	Upper decision threshold	[0.8, 0.95]
$\underline{B}$	x_5	Lower decision threshold	[0.05, 0.2]
$\mathcal{M}(0)$	x_6	Initial target probability map	{good, bad, none}
SP	x_7	Exhaustive search pattern	{lawnmower, sweeping}

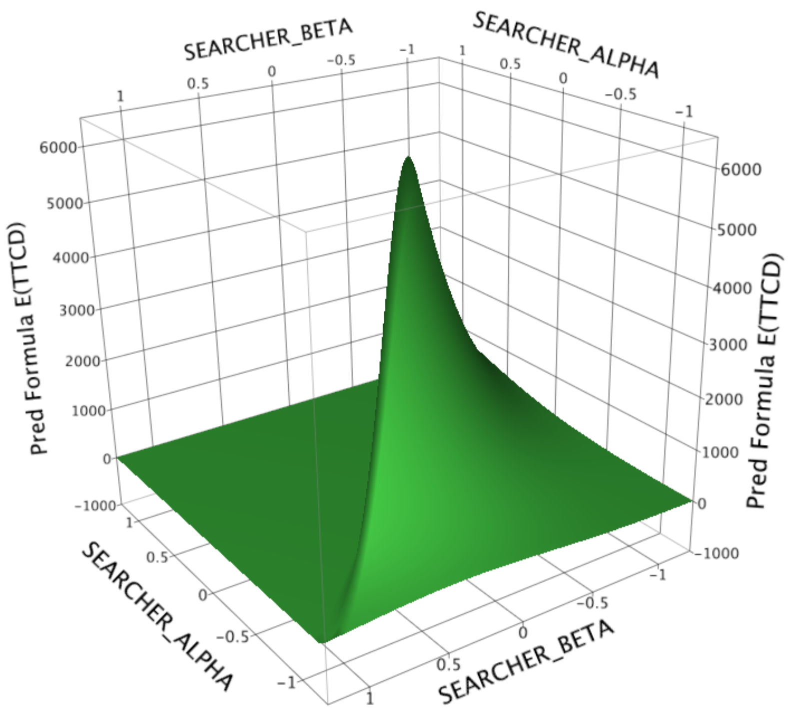
- A picture of the hybrid D-optimal and uniform design in two of the factors is illustrated as

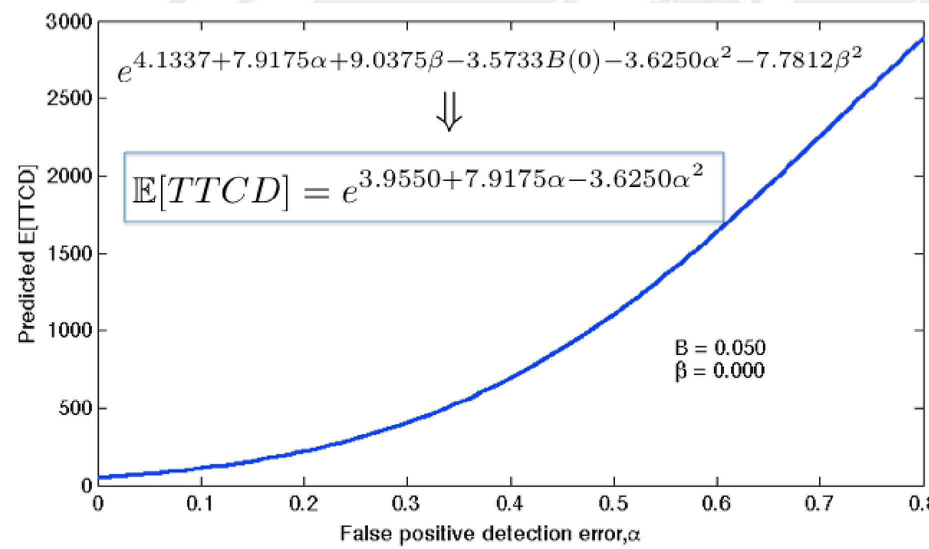




Results

Lawnmower	Factors														
		Main Effects							Interactions					Squared Effects	
						x_6				x_1x_6					
Response	Intercept	x_1	x_2	x_3	x_5	*bad*	*good*	*none*	x_1x_3	*bad*	*good*	*none*	x_3x_5	x_1^2	x_2^2
% Correct Neg	-0.147	-0.172		-0.888											
% Correct Pos	-0.917	-0.094		1.163	-0.404	-0.657	0.330	0.330		-0.436	0.198	0.238	0.271		
E[TTCD]*	8.644	2.007	1.125		-0.268									-0.580	-1.245
E[TTCND]*	8.462	1.800	1.175	0.415	-0.319										-1.541
E[TTCPD]*	8.737	2.262	0.961	0.110					-0.278					-0.533	-1.549





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