Technical Risk Reduction: Sequential Design of Experiments and Uncertainty Quantification

CCSI²
Carbon Capture Simulation for Industry Impact

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Design of Experiments (DoE)

- Mathematical strategy for selecting input combinations to estimate or observe an output
- Make purposeful changes to inputs to identify the reasons for any changes in output
- A well-designed experiment is critical for drawing conclusions

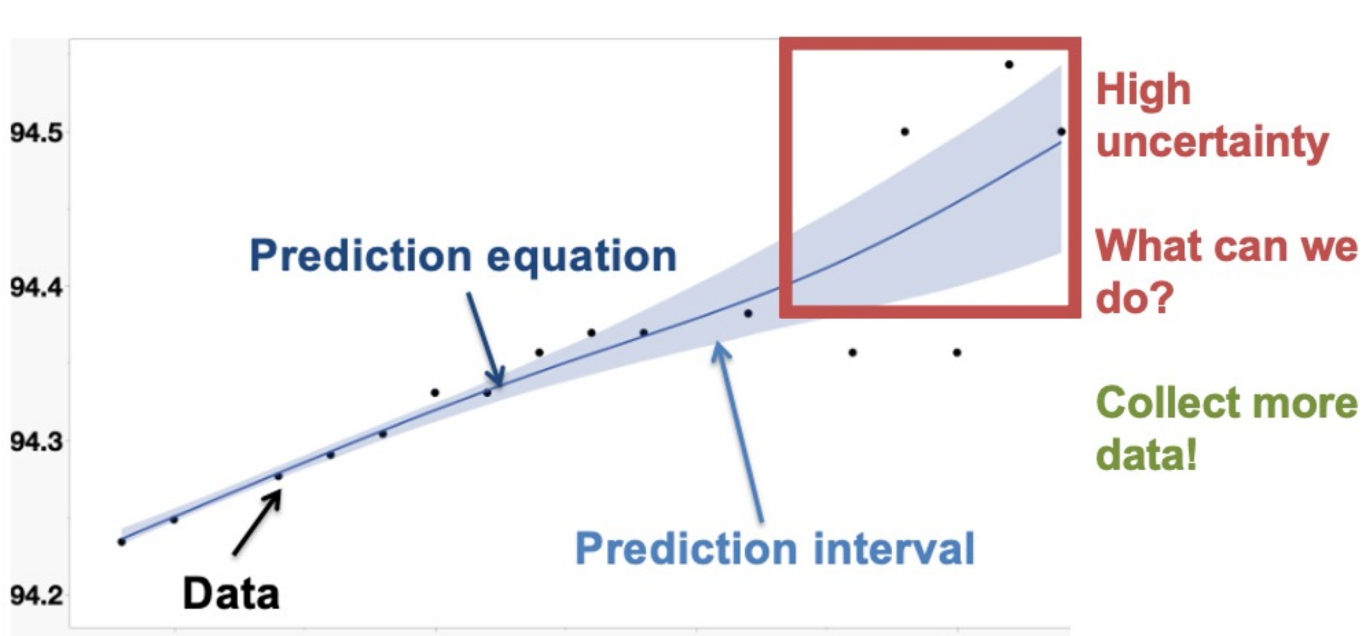
Proven track record of maximizing performance, minimizing risk

- Maximize learning with a fixed budget
- Saved 2 years and \$2-3M off pilot testing
- Over 25% reduction in model uncertainty
- CO_2 Capture percentage within 3-6% with 95% confidence

- Use DoE to gain key insights for development and improvement
  - Strategic data collection + model estimation
- But: All models contain some level of uncertainty
  - Form of the model, values of model parameters, experimental data used

Uncertainty Quantification (UQ)

- UQ: collection of statistical methods to characterize, estimate, understand model uncertainty
- Crucial for targeting and reducing sources of uncertainty



Sequential DoE (SDoE)

- SDoE: Directly incorporate knowledge learned in previous stages
- Strategic data collection across multiple stages; reduce resources needed and reduce risk

Feasibility study	Exploration of input space	Model building / refinement	Optimization	Confirmation
Is it possible to collect quality data? Proof of concept	Understand basic relationship between inputs and responses	Verify that the model captures patterns. Add data for better model parameter estimation or prediction	Focus on region of maximum interest. Close to most desirable operation conditions	Verify results for production or operational use. Ability to reproduce results

Success Stories

MTR FIELD TEST AT TCM

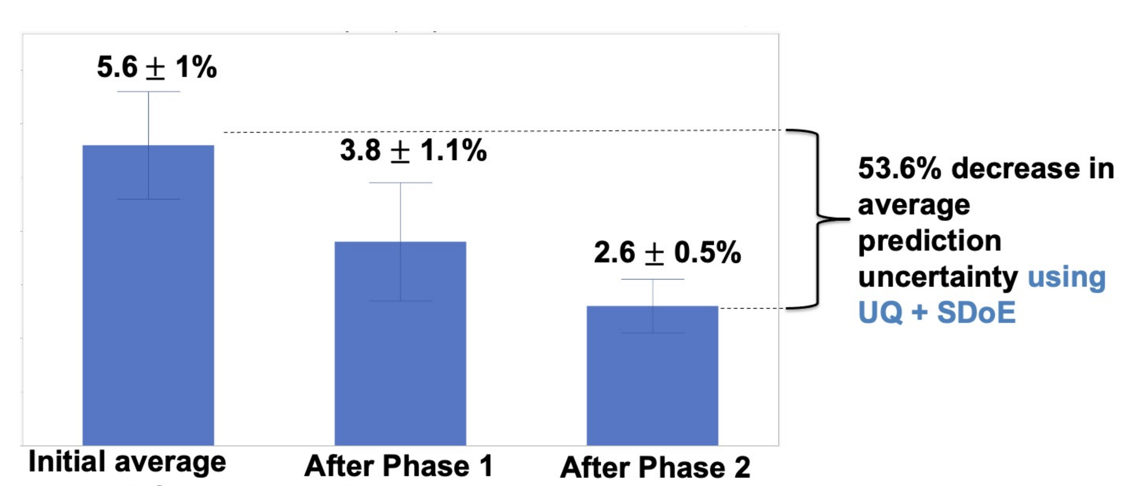
- CCSI² supported Membrane Technology and Research engineering-scale advanced membrane field test at Technology Centre Mongstad (TCM)

- CCSI² Team leveraged UQ and SDoE tools to make the most of the experimental budget – Learn as we go, increase efficacy

RTI TEST CAMPAIGN AT TCM

- CCSI² supported Research Triangle Institute test campaign for NAS solvent system at TCM
- Leveraged SDoE to meet objectives while accounting for flexibility in schedule

AQUEOUS MEA PILOT PLANT CAMPAIGN AT NCCC



CCSI² SDoE Capabilities

SPACE-FILLING DESIGNS

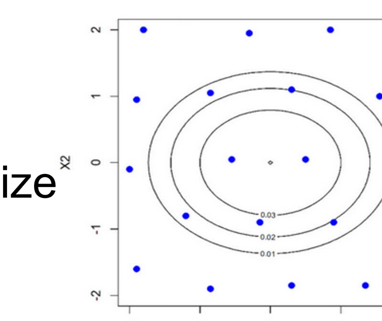
Relationship between inputs and response of interest not well-understood

- MaxiMin Designs: maximize the minimum distance between any pair of design points in the design space
  - Use for exploration

$$d(\boldsymbol{x}_1, \boldsymbol{x}_2) = \sqrt{\sum_{j=1}^{p} (x_{1j} - x_{2j})^2}$$

The Euclidean distance between any two points in the design space $\mathcal{X}^p$

A maximin design of size n, denoted $D_{Mm}(n)$



$$D_{Mm}(n) = \max_{D_n \subset \mathcal{X}^p} \min_{\boldsymbol{x}_i, \boldsymbol{x}_{i'} \in D_n} d(\boldsymbol{x}_i, \boldsymbol{x}_{i'})$$

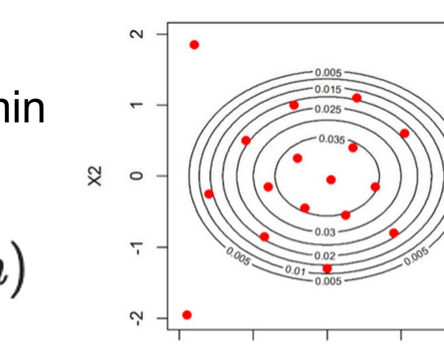
- Non-Uniform MaxiMin Designs: A weighted MaxiMin design
  - Use for uncertainty reduction

$$d^w(\boldsymbol{x}_1, \boldsymbol{x}_2) = \sqrt{w(\boldsymbol{x}_1) w(\boldsymbol{x}_2) d(\boldsymbol{x}_1, \boldsymbol{x}_2)^2}$$

The weighted distance between any two points in the design space

$w(\boldsymbol{x})$ is the weight associated with a design point $\boldsymbol{x} \in \mathcal{X}^p$

A weighted maximin design of size n, denoted $D^w_{Mm}(n)$

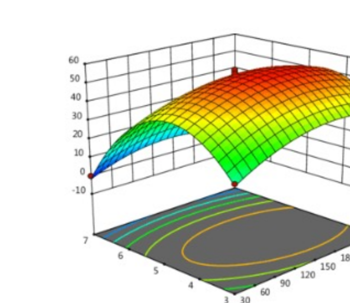


$$D^w_{Mm}(n) = \max_{D_n \subset \mathcal{X}^p} \min_{\boldsymbol{x}_i, \boldsymbol{x}_{i'} \in D_n} d^w(\boldsymbol{x}_i, \boldsymbol{x}_{i'})$$

MODEL-BASED OPTIMAL DESIGNS

When relationship between inputs and response of interest can be well-approximated by a low-order polynomial

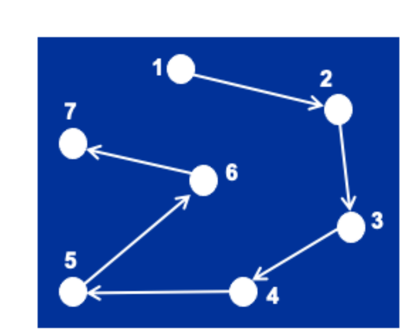
- Use for initial exploration
  - To refine experimental scope
  - When process model is under development



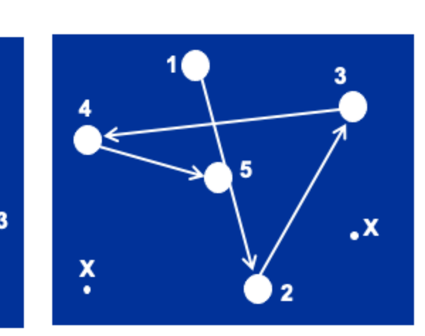
A Ψ - optimal design of size n, denoted by $\xi^*_\Psi(n)$

$$\xi^*_\Psi(n) = \arg\min_{\mathbf{x} \in \mathcal{X}^p} \Psi\{M(\xi(n))\} \text{ where } M(\xi(n)) = \frac{1}{\sigma^2} \sum_{i \le p} n_i \mathbf{x}_i \mathbf{x}_i'$$

EFFICIENT IMPLEMENTATION OF EXPERIMENTAL RUN ORDER



Ordered



Unordered

- Order to efficiently reach equilibrium
- Allow for maximum number of runs within a constrained timeline
- Comes with trade-offs, but can allow larger, non-randomized experiment

CCSI²: Experts to talk to and work with

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