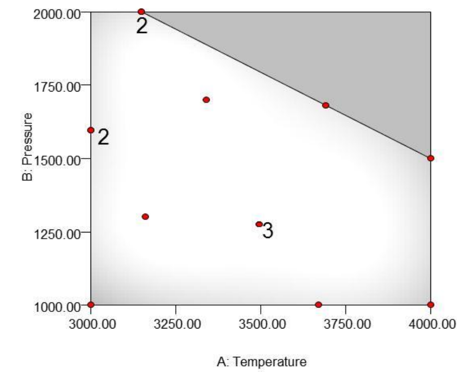


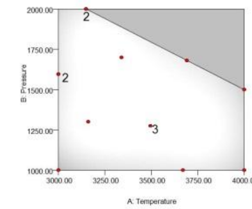
Practical Aspects for Designing Statistically Optimal Experiments

from an engineer's perspective

Mark J. Anderson, PE
Stat-Ease, Inc.
mark@statease.com

Pat Whitcomb
Stat-Ease, Inc.

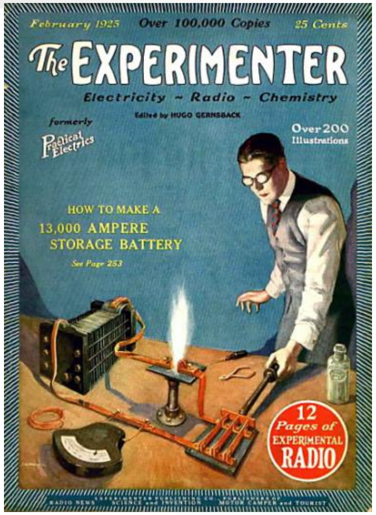
Agenda



- What's required for a good design.
- Optimal point selection (*IV versus D optimality*).
- Practical aspects algorithmic design.
- Optimal design example.
- Conclusion and recommendations.

Study Considerations

An Experimenter’s (Practical) View



- What is the objective of the study?
- State the objective in terms of measured responses:
  - How will the responses be measured?
  - What precision is required?
- Which factors will be studied?
- What are the regions of interest and operability?
- How will the response behave—linear or curvy?
- What design should we use?

"Good" Response Surface Designs
A Statistician's Checklist

- ✓ Allow the chosen polynomial to be estimated well.
- ✓ Give sufficient information to allow a test for lack of fit.
  - ❖ Have more unique design points than coefficients in model.
  - ❖ Provide an estimate of "pure" error.
- ✓ Be insensitive (robust) to the presence of outliers in the data.
- ✓ Be robust to errors in control of the factor levels.
- ✓ Permit blocking and sequential experimentation.
- ✓ Provide a check on homogeneous variance assumption and other useful model diagnostics; including deletion statistics.
- ✓ Generate useful information throughout the region of interest, i.e., provide a good distribution of standard error of prediction.
- ✓ <u>Not contain an excessively large number of runs</u>.

"Good" Response Surface Designs

Comments on the Checklist

Re: Pitfalls of Optimality:

"Souped-Up Car Syndrome:

Optimize speed and produce a delicate gas-guzzler."

Peter J. Huber*

"Designing an experiment should involve balancing multiple objectives, not just focusing on a single characteristic."

Myers, Montgomery and Anderson-Cook**

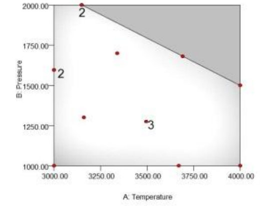
"Alphabetic optimality is not enough!"

Pat Whitcomb

* "On the Non-Optimality of Optimal Procedures" *Optimality: Lehmann Symposium*, Institute of Mathematical Statistics, 2009, 31-46.

** *Response Surface Methodology, 3rd Ed*, Wiley, 2009.

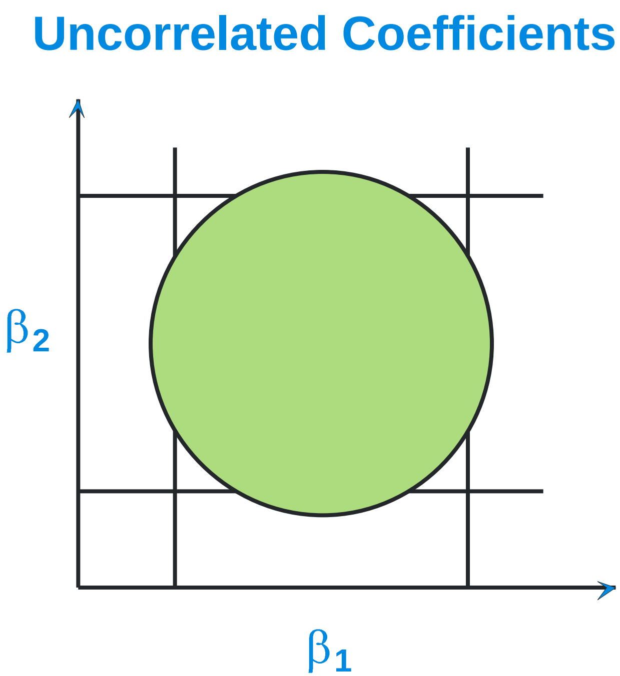
Agenda

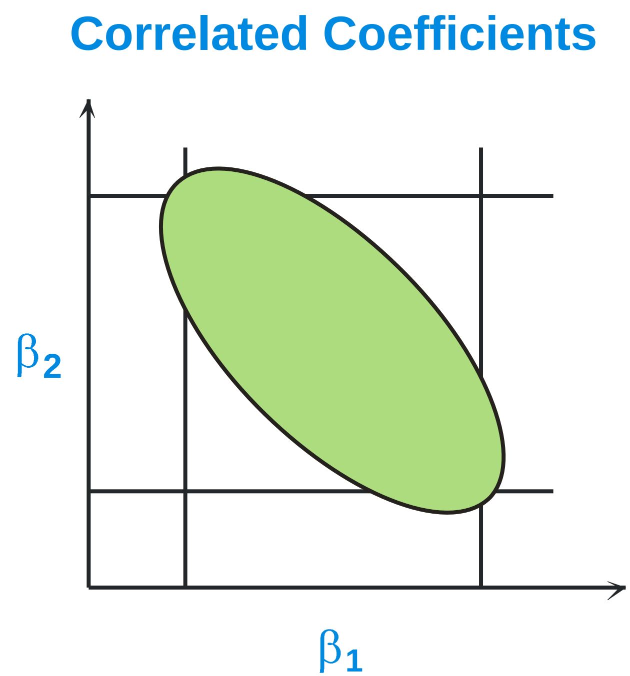


- ✓ What’s required for a good design.
- ❑ **Optimal point selection (*IV versus D optimality*).**
- ❑ Practical aspects algorithmic design.
- ❑ Optimal design example.
- ❑ Conclusion and recommendations.

D-optimal Point Selection

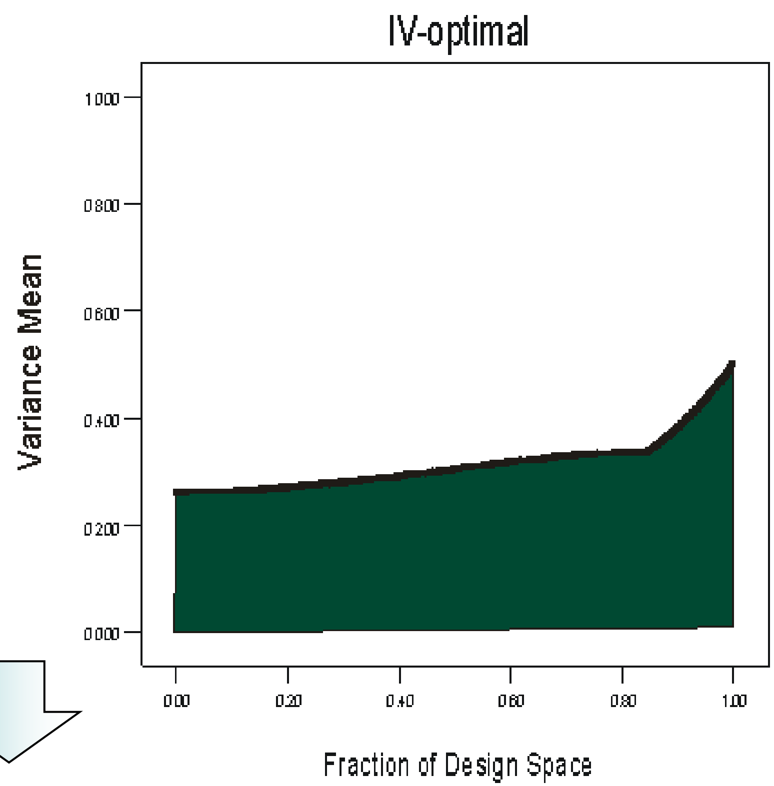
Goal: D-optimal design minimizes the determinant of the $(X'X)^{-1}$ matrix. This minimizes the volume of the confidence ellipsoid for the coefficients and maximizes information about the polynomial coefficients.





Optimal Point Selection
IV-optimal Point Selection

An IV-optimal design seeks to minimizes the integral of the prediction variance across the design space. These designs are built algorithmically to provide lower integrated prediction variance across the design space. This equates to minimizing the area under the fraction of design space (FDS) curve.

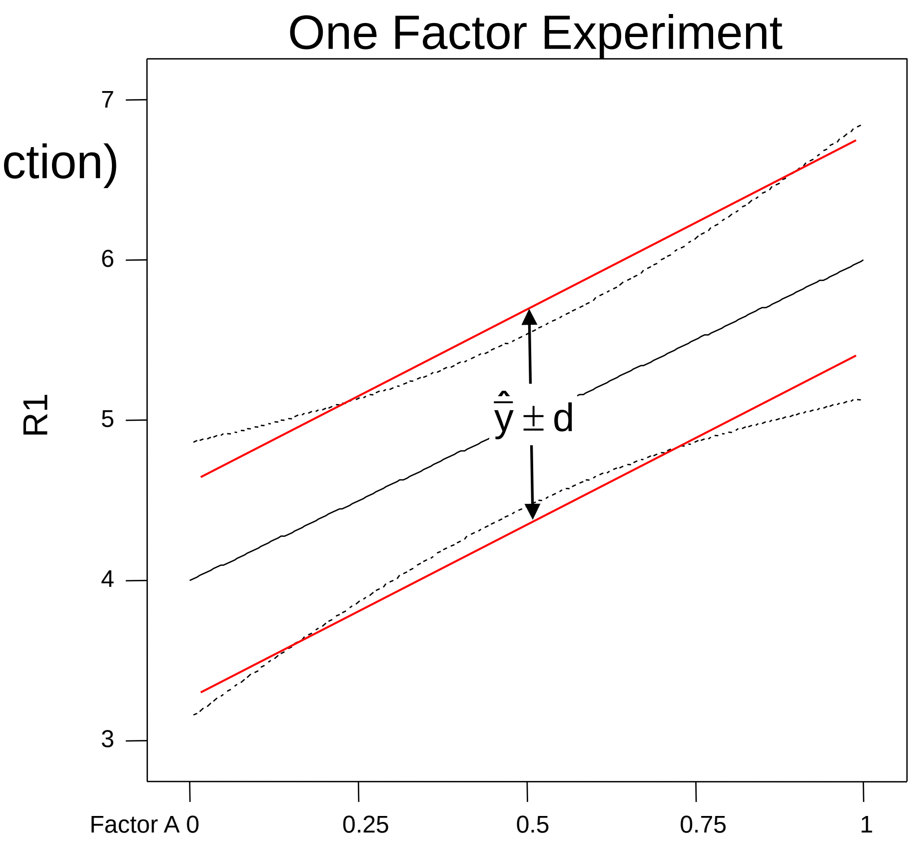


What's in this for you?
See following three slides.

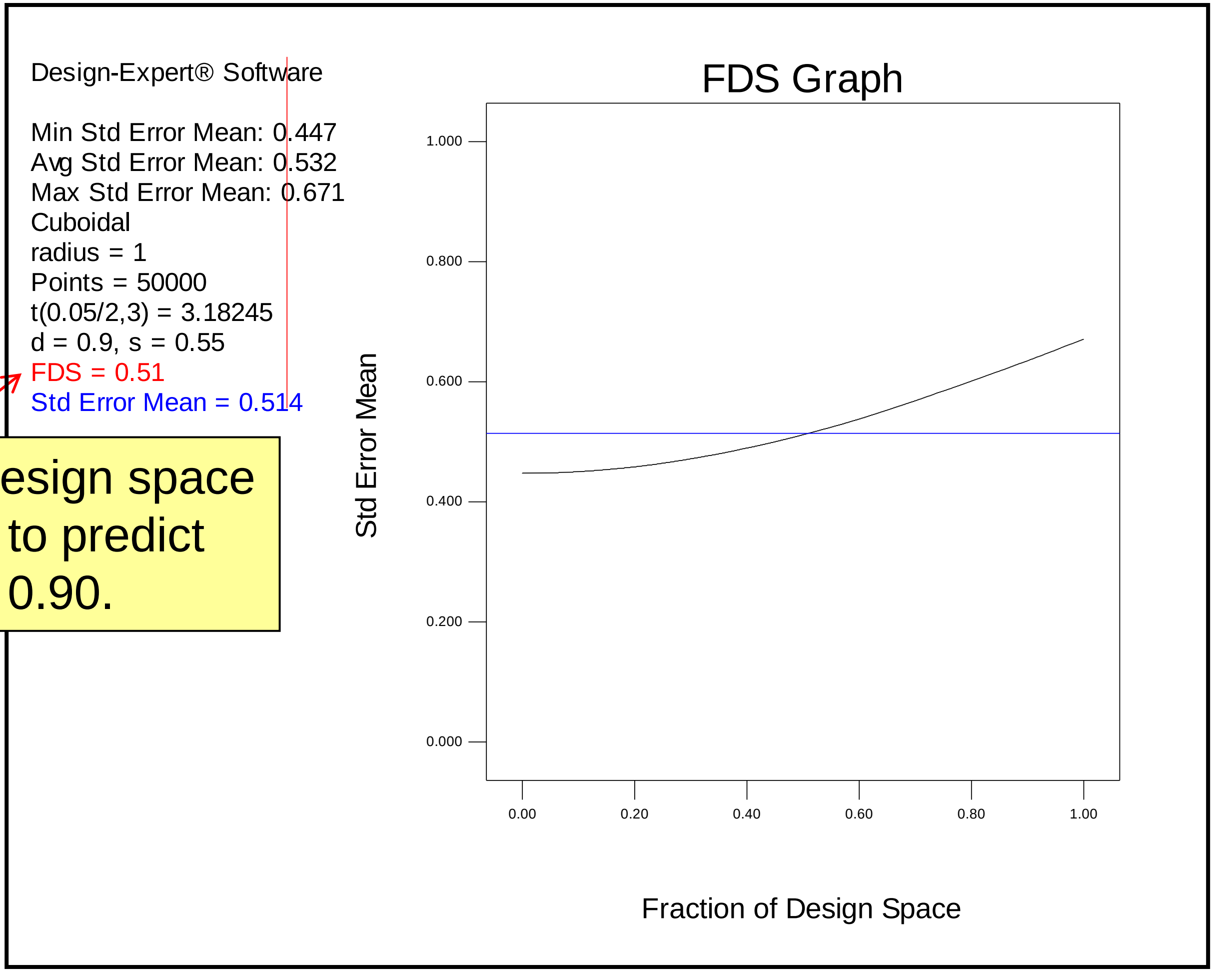
Primer on FDS
One Factor *(part 1 of 2)*

- Solid center line is fitted model
- $\hat{y}$ is expected value (mean prediction)
- Curves are confidence limits (actual precision)
- d is half-width of the desired CI (desired precision)—it creates the red lines.

Note: The actual precision of the fitted value depends on where we are predicting.

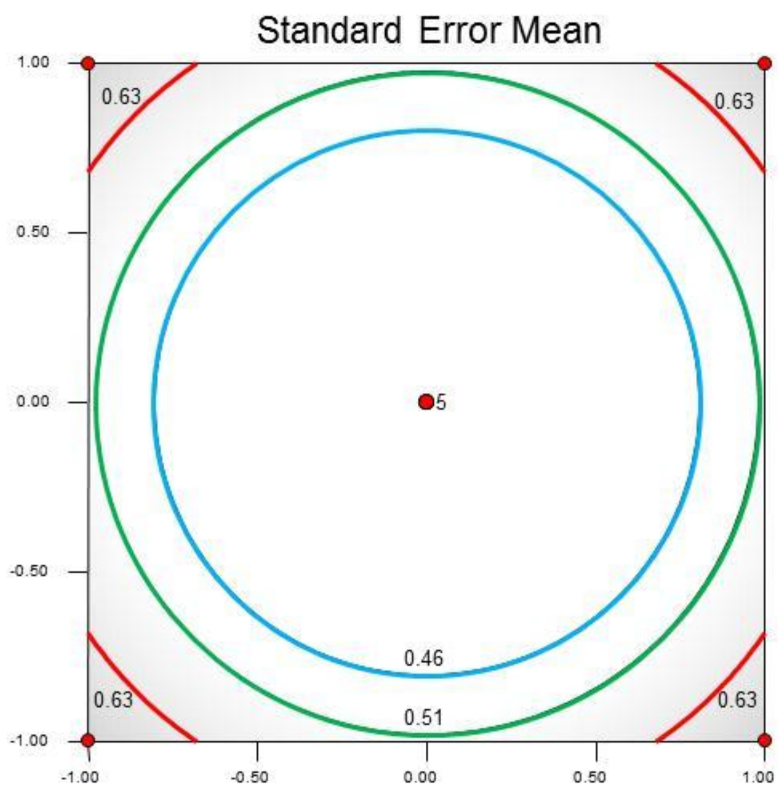


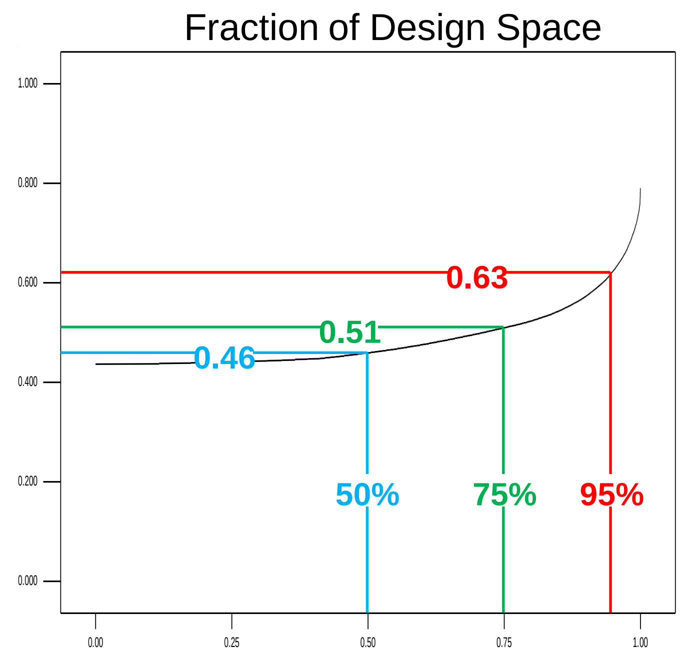
Primer on FDS
One Factor *(part 2 of 2)*



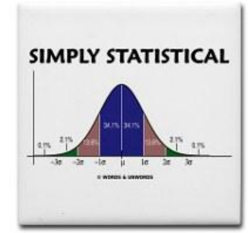
Only 51% of the design space is precise enough to predict the mean within ± 0.90.

Primer on FDS
Two Factor





Optimal Point Selection
IV versus D Optimal Design

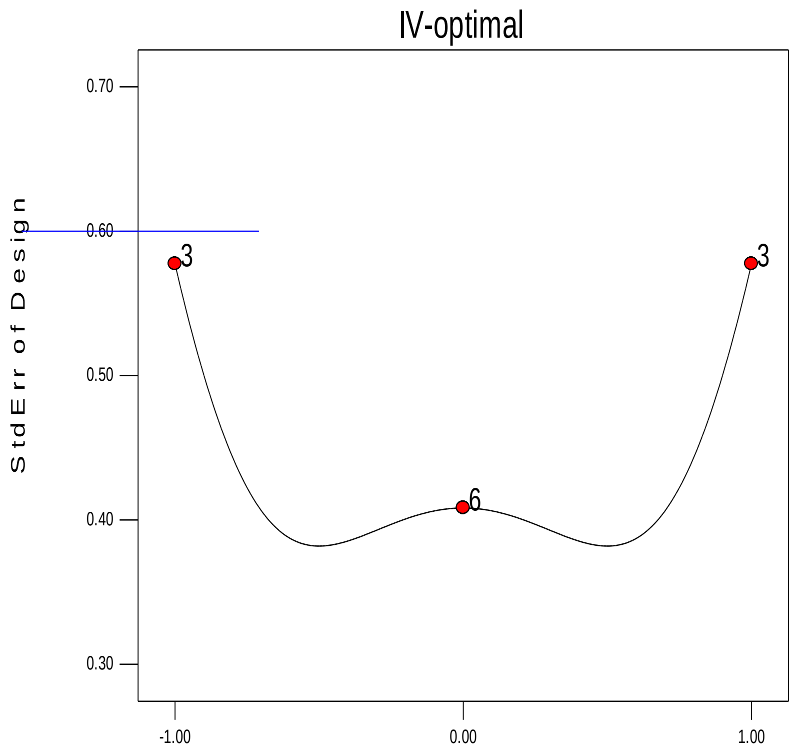


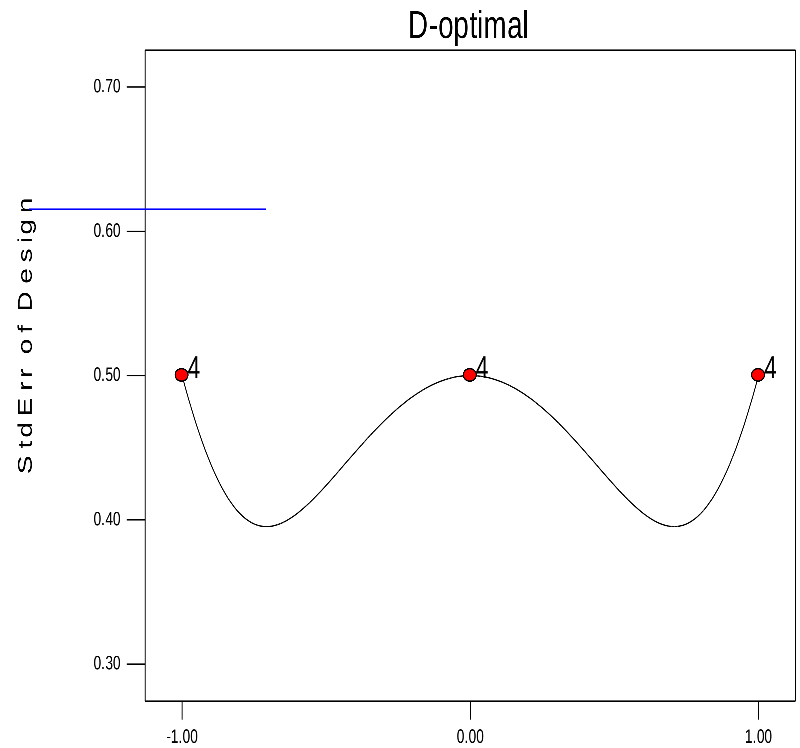
Compare point selection using IV-optimal and D-optimal:

- Build a one factor design.
- Design for a quadratic model.
- Choose 12 runs using optimality as the only criterion.

IV versus D Optimal Design

Optimal 12 Point Designs

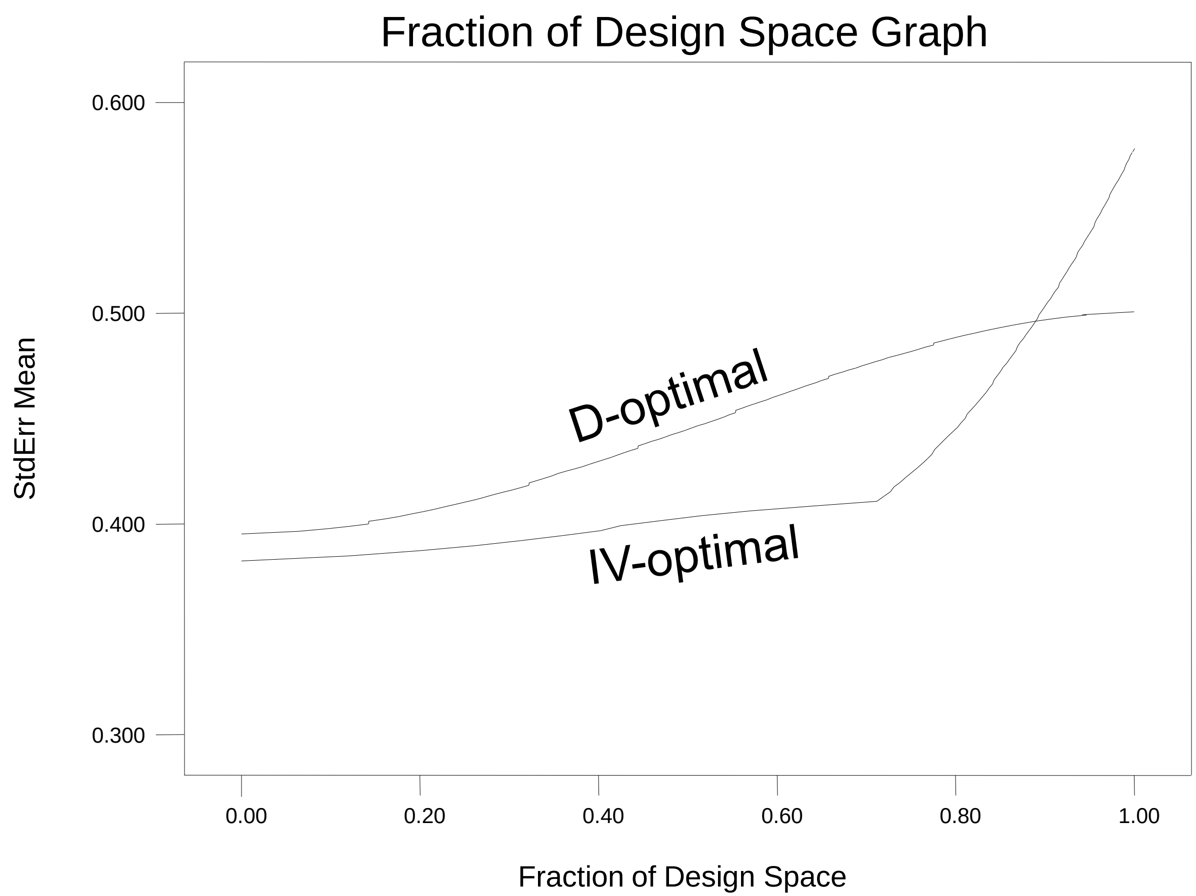




Compare and contrast.

IV-optimal versus D-optimal

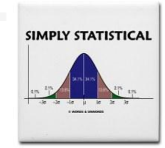
One Factor 12 Optimal Points



IV min:	0.382
IV avg:	0.421
IV max:	0.577
D min:	0.395
D avg:	0.447
D max:	0.500

Compare and contrast.

What about G-Optimality?
Three 6-Point 2-Factor Designs



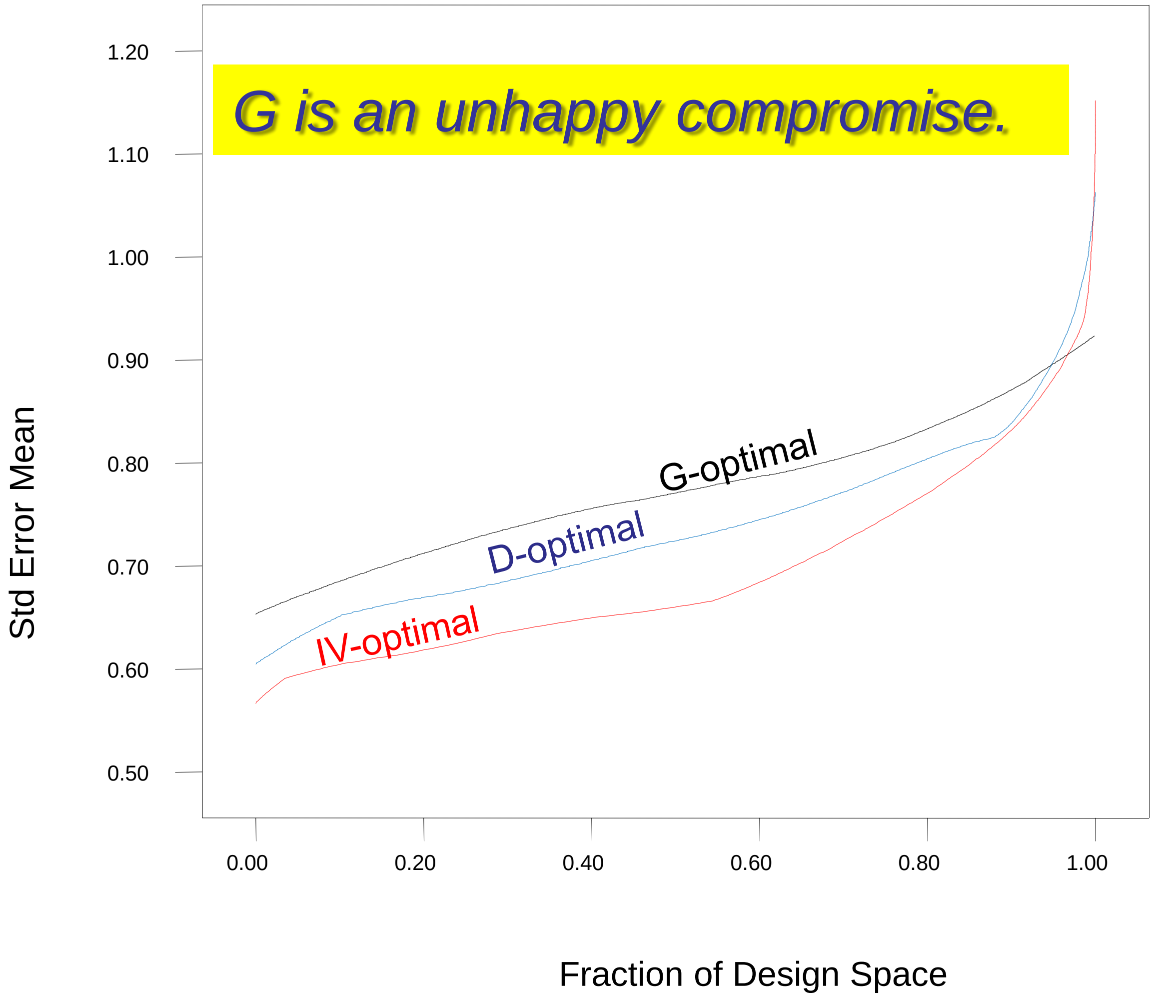
	G-optimal	D-optimal	IV-optimal
G efficiency	87.9%	66.4%	56.5%
Min SE mean	0.653	0.604	0.566
Ave SE mean	0.777	0.743	0.699
Max SE mean	0.923	1.063	1.152

G-optimal designs:

- Minimize the maximum predicted variance.
- This is at the expense of the average prediction variance.
- For a gain in a very small fraction of the design space, precision is sacrificed in the vast majority of the design space. *(see next slide)*

What about G-Optimality?

Three 6-Point 2-Factor Designs



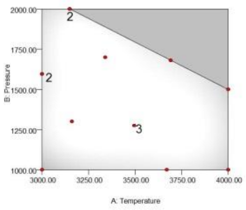
Optimal Point Selection

IV versus D Optimal Design

<u>Conclusions</u>:

- IV-optimal designs tend to place points more uniformly in the design space.
- IV-optimal designs have a higher maximum prediction variance; therefore a lower G-efficiency.
- IV-optimal designs have a lower average prediction variance. *(This also contributes to a lower G-efficiency.)*
- **Being minimum level designs neither IV nor D can evaluate sufficiency of quadratic model! They must be augmented to test lack of fit.**

Agenda



- ✓ What's required for a good design.
- ✓ Optimal point selection (*IV versus D optimality*).
- ❑ **Practical aspects algorithmic design.**
- ❑ Optimal design example.
- ❑ Conclusion and recommendations.

Optimal Point Selection

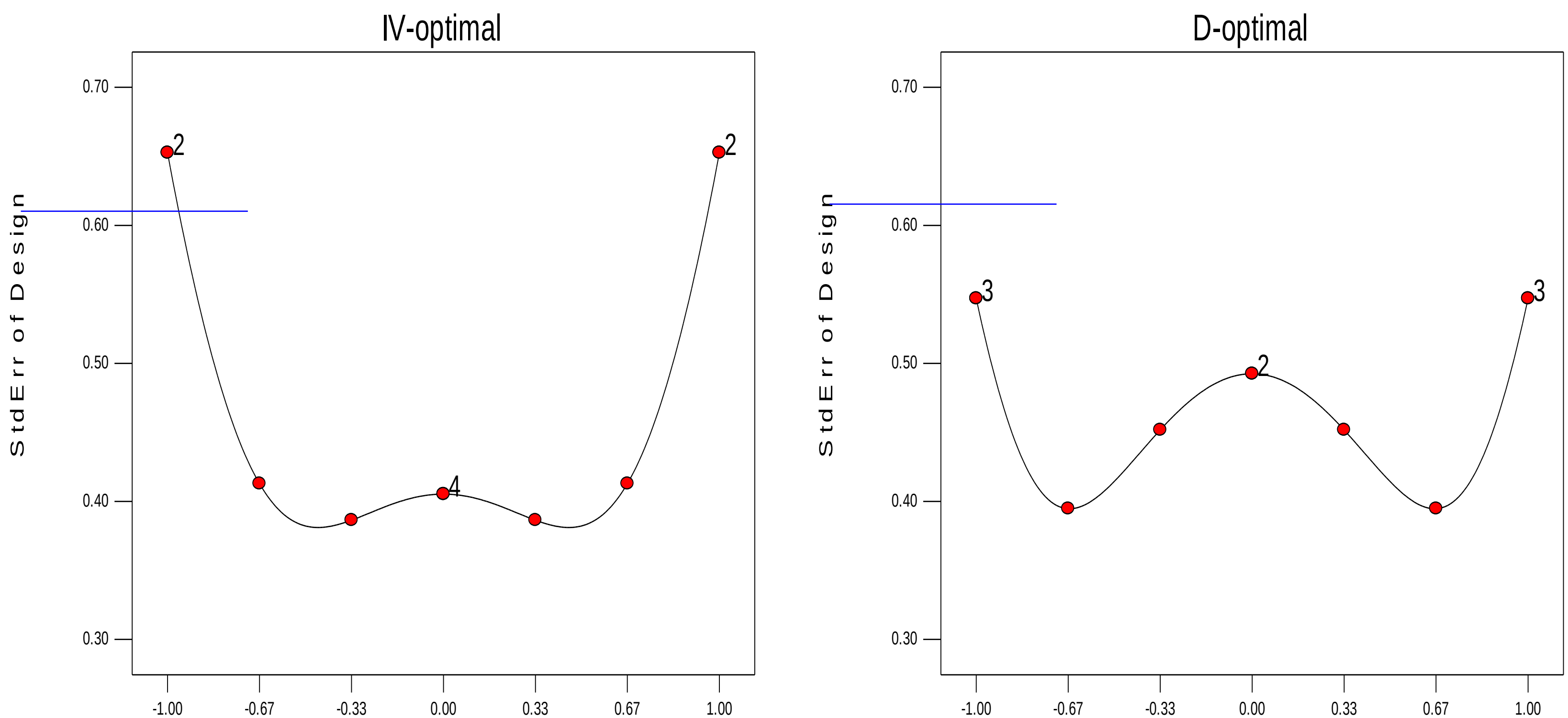
IV versus D Optimal Design

Compare point selection using IV-optimal and D-optimal :

- Build a one-factor design.
- Design for a quadratic model.
- Choose **eight** of the twelve runs using optimality as the criteria.
- Choose **four** of the twelve runs as lack of fit (LOF) points using distance as the criteria.
  (Maximize the minimum distance from an existing design point; i.e. fill the “holes”.)

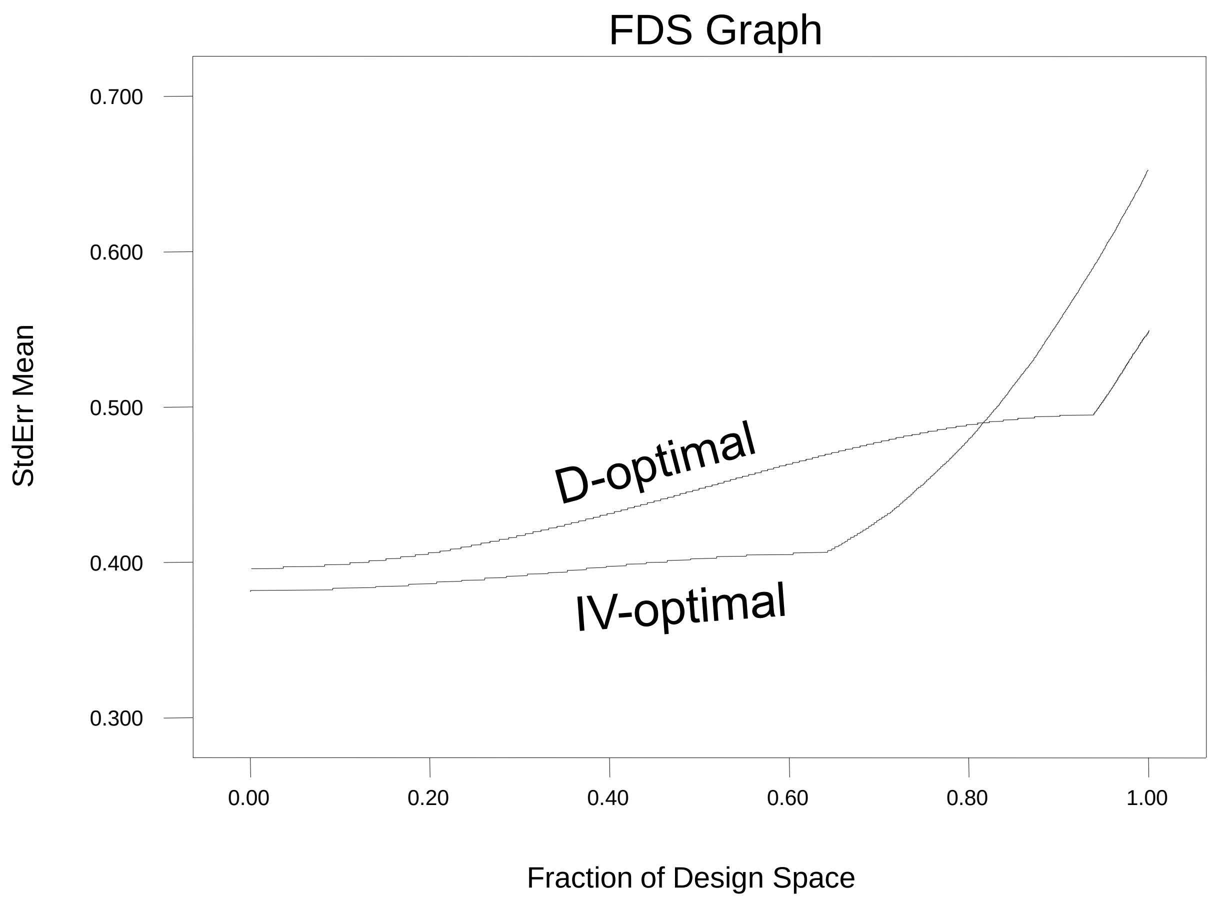
Optimal Designs

8 Optimal + 4 LOF Points



IV-optimal versus D-optimal

One-Factor Design, 8 Optimal + 4 LOF Points

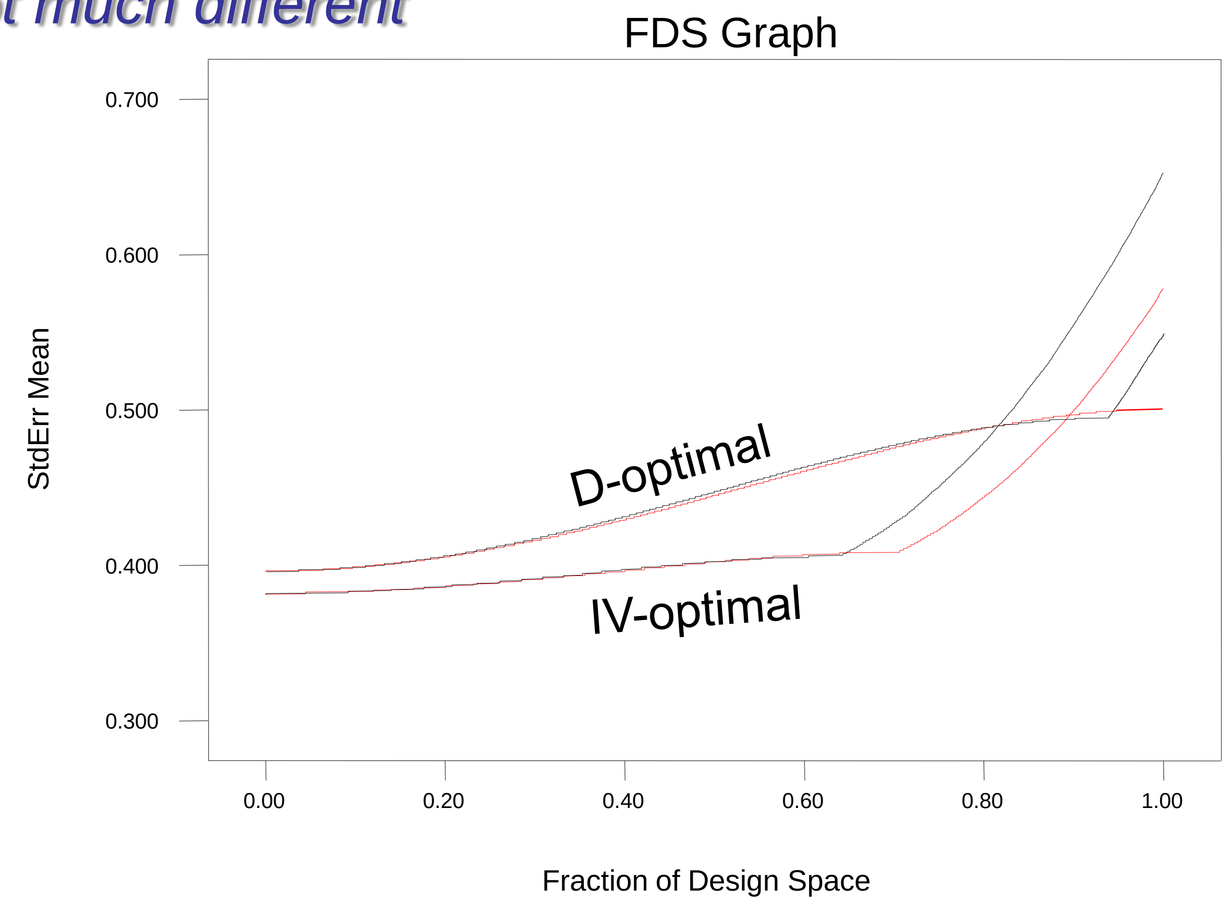


IV min:	0.381
IV avg:	0.438
IV max:	0.653
D min:	0.395
D avg:	0.448
D max:	0.547

IV-optimal versus D-optimal

12 Optimal (no LOF) vs 8 Optimal + 4 LOF

Not much different



8 opt + 4 dist

IV min:	0.381
IV avg:	0.438
IV max:	0.653
D min:	0.395
D avg:	0.448
D max:	0.547

12 optimal

IV min:	0.382
IV avg:	0.421
IV max:	0.577
D min:	0.395
D avg:	0.447
D max:	0.500

Optimal Point Selection

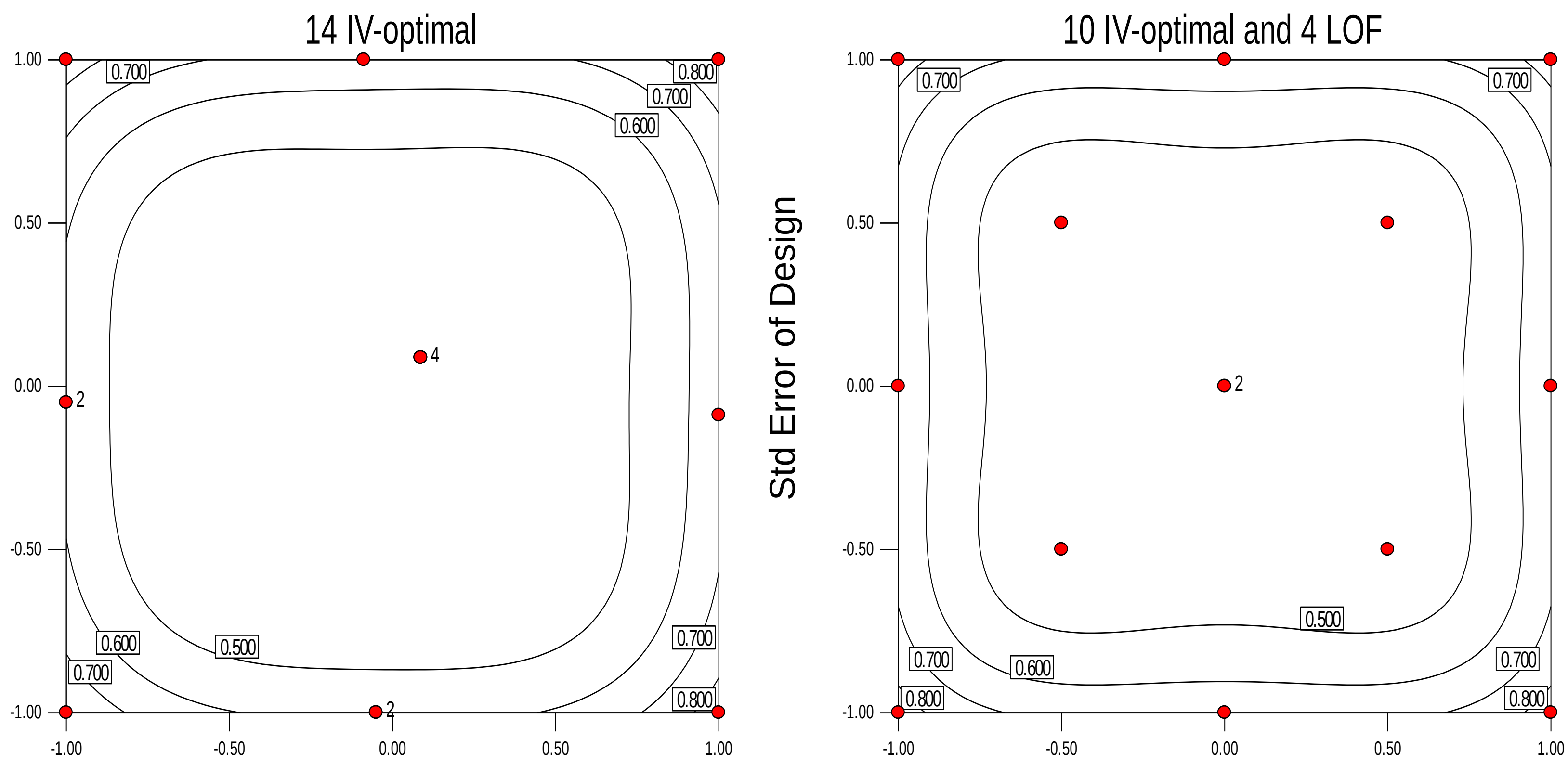
IV versus D Optimal Design

Compare point selection for a two-factor 14-run design:

- Design for a quadratic model.
- IV-optimal:
  - 14 optimal runs (no LOF)
  - 10 optimal and 4 LOF *(distance)*
- D-optimal:
  - 14 optimal runs (no LOF)
  - 10 optimal and 4 LOF *(distance)*

IV-optimal Designs

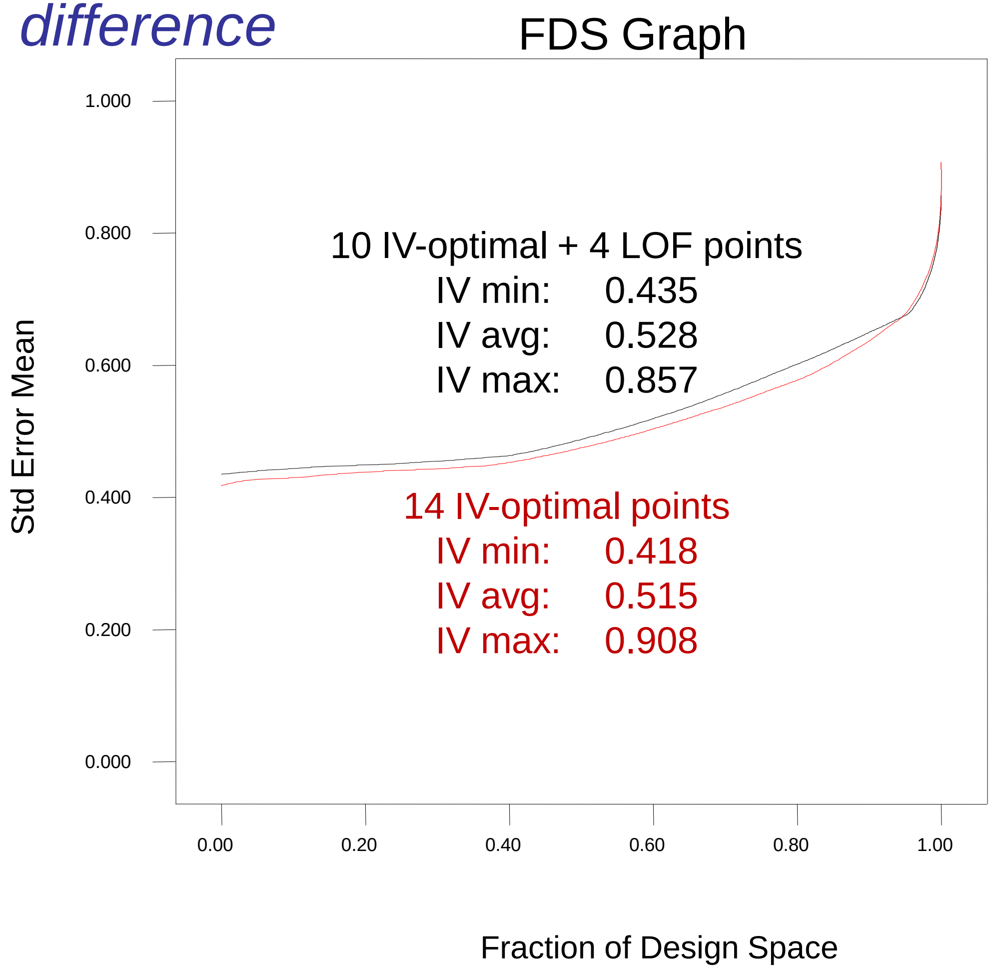
14-Run Designs with 0 vs 4 LOF Points



IV-optimal Designs

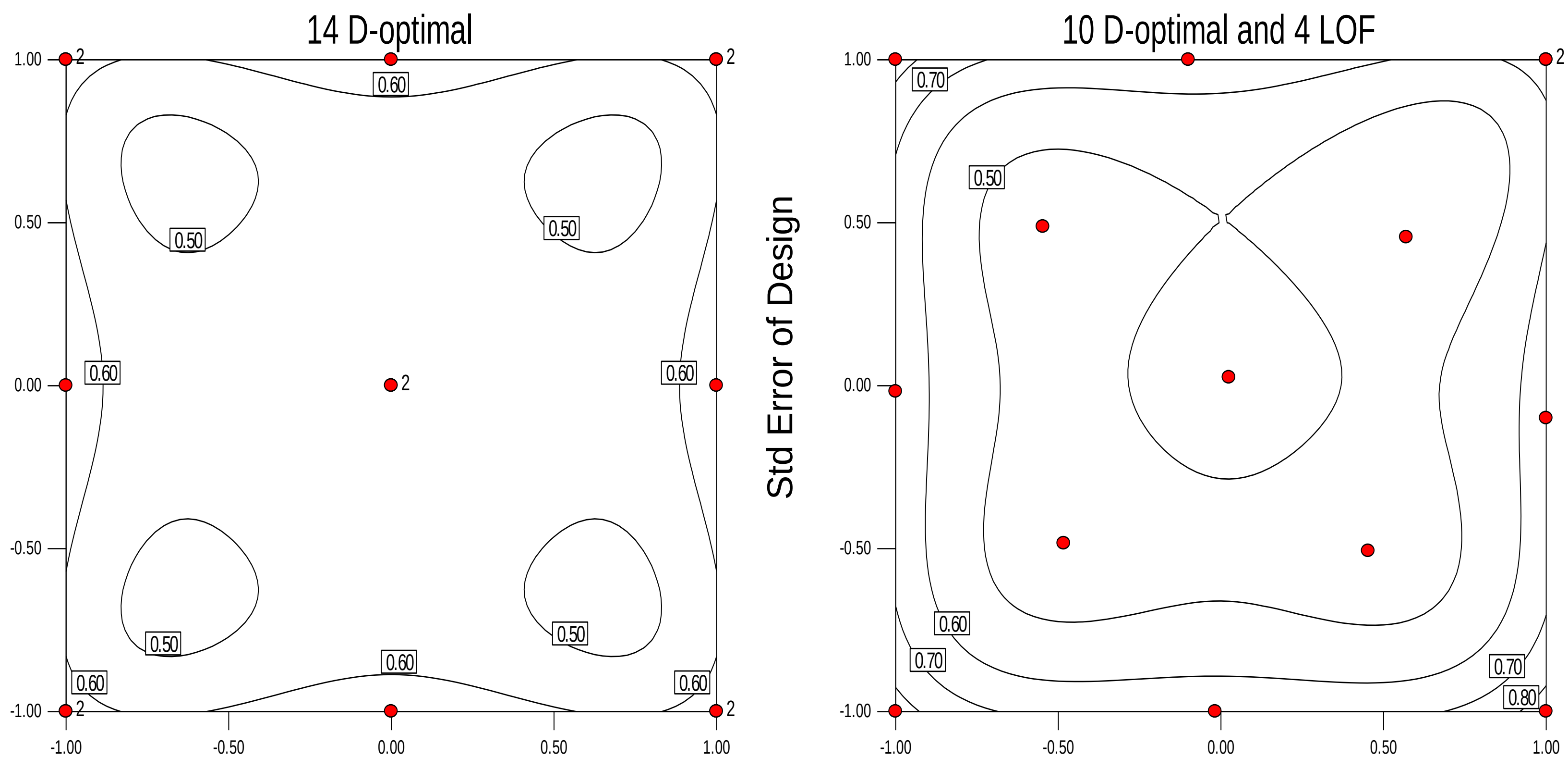
14-Run Designs with 0 vs 4 LOF Points

Not much difference



D-optimal Designs

14-Run Designs with 0 vs 4 LOF Points

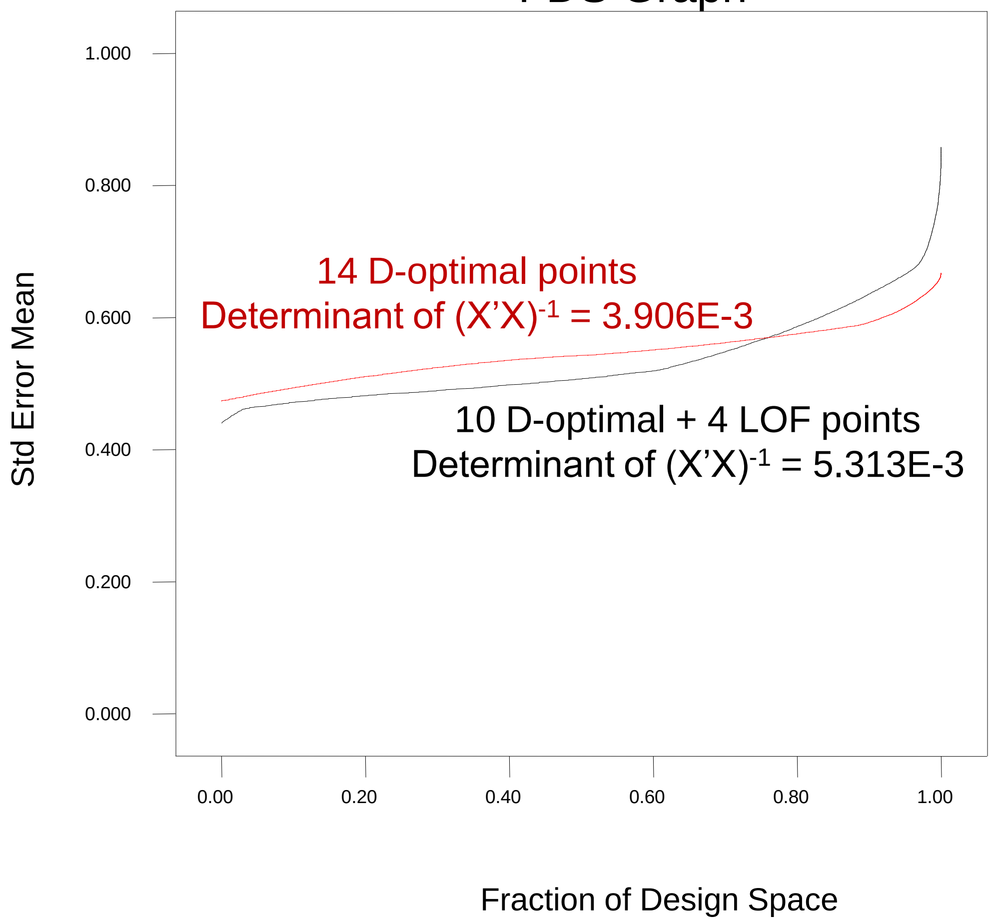


D-optimal Designs

14 Run Designs with 0 and 4 LOF Points

Not much difference

FDS Graph



Practical Aspects Algorithmic Design

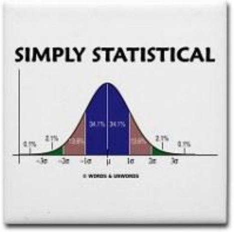
Lack of Fit Points

Adding LOF points:

- The design is not as alphabetically optimal but only slightly off-kilter on FDS plot (not much difference).
- Ability to detect lack of fit is enhanced.
- <u>Adding LOF points is a good trade off</u>!

Practical Aspects Algorithmic Design

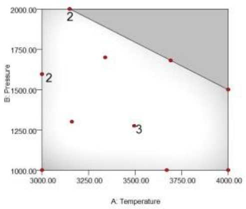
Pure Error Estimation



Estimating pure error:

- In physical experiments it is desirable build in an estimate of experimental error—just so you know.
- Replicates provide an estimate of experimental error independent of model assumptions. They allow for a test on lack of fit.
- <u>Adding replicates is a good tradeoff</u>!

Agenda



- ✓ What's required for a good design.
- ✓ Optimal point selection (*IV versus D optimality*).
- ✓ Practical aspects algorithmic design.
- ❑ **Optimal design example.**
- ❑ Conclusion and recommendations.

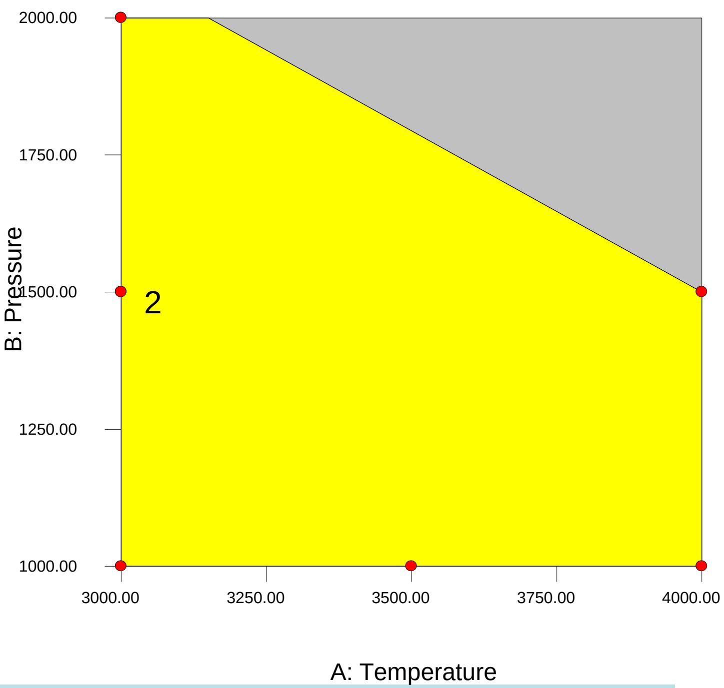
Optimal Design: Aerospace Example*

Aerospace engineers tested a freejet nozzle's exit profile at:

A. Temperature, low to high.

B. Pressure, low to high.

The experiment design required an upper constraint to avoid both factors being at their high levels. It is a minimal-run D-optimal with one point replicated.

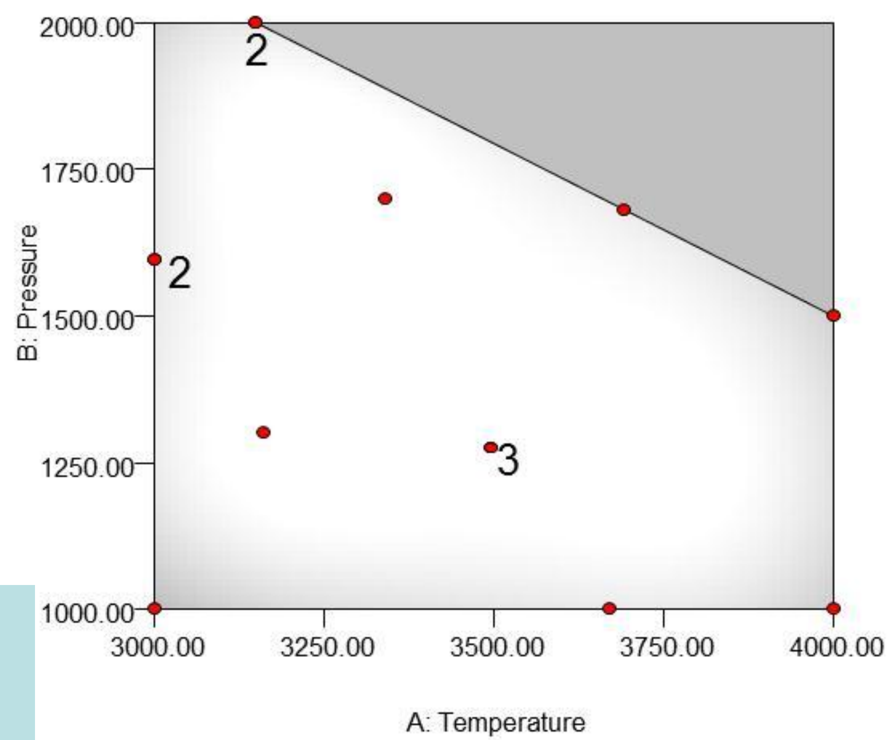


**(Based on "Developing, Optimizing and Executing Improved Test Matrices," Dusty Vaughn & Doug Garrard, USAF T&E Days 2009.)*

Optimal Design: Aerospace Example

An Alternative Design

This stouter design* features 4 more points for lack-of-fit plus 4 points replicated for a stronger estimate of pure error. Also, the optimality criterion for this design is IV—now favored for RSM designs (vs the D-optimal in vogue at the time of this experiment).

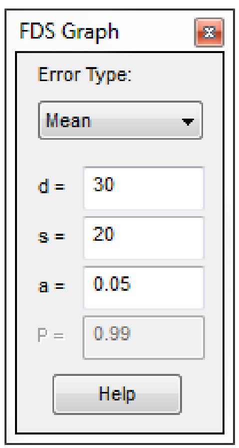


(Detailed in "How to Frame a Robust Sweet Spot via Response Surface Methods", 2010 NDIA T&E Conf talk by MJA.)

Aerospace Example
Evaluate your IV-optimal Design

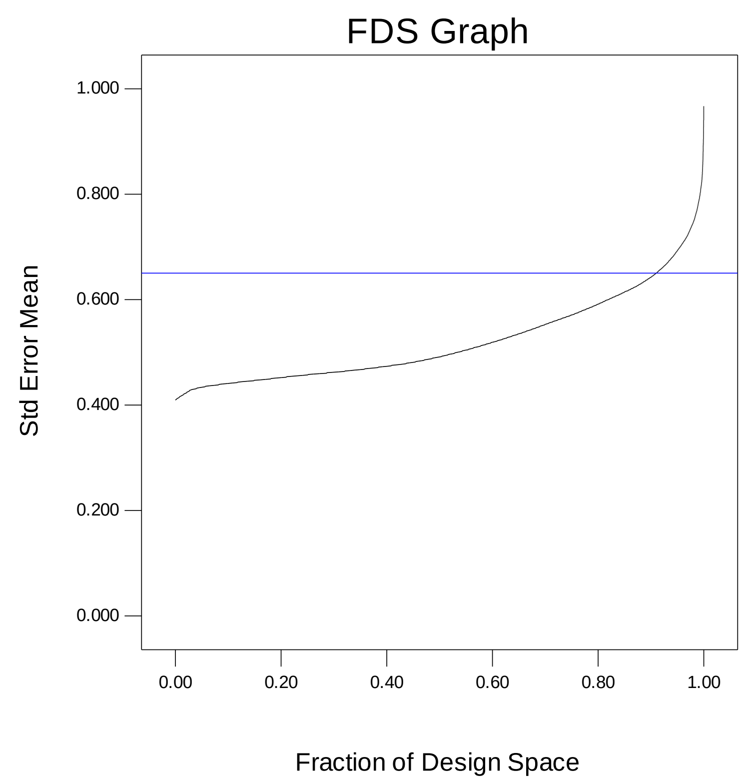
Is the stouter optimal design precise enough?

- Assume standard deviation of 20 for the prime response.
- ✓ Then a difference "d" of 30 will likely be detected.*
  (Versus ~260 for the near-minimal D-optimal design!)

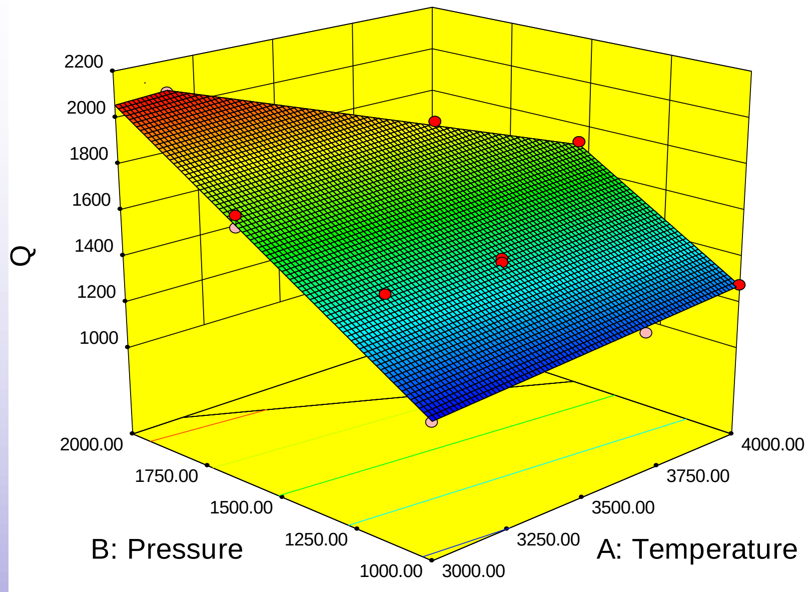


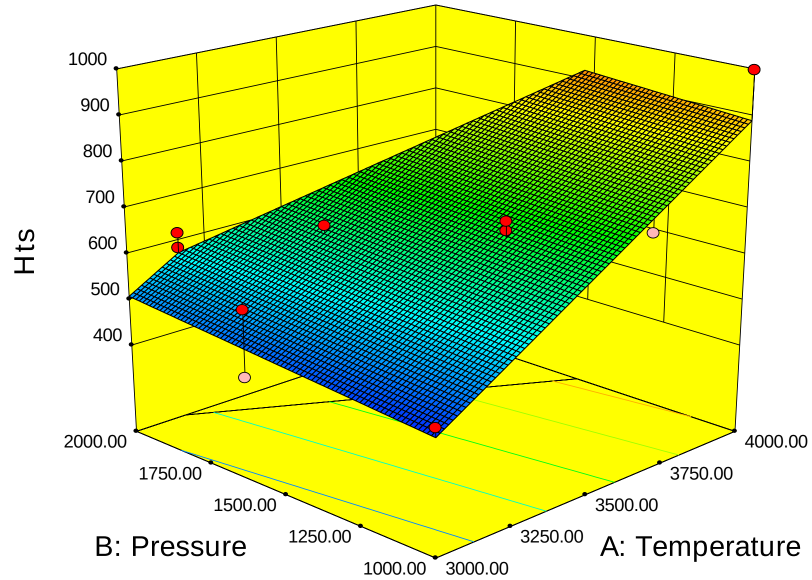
Design-Expert® Software

Min Std Error Mean: 0.409
Avg Std Error Mean: 0.528
Max Std Error Mean: 0.967
Constrained
Points = 50000
t(0.05/2,8) = 2.306
d = 30, s = 20
FDS = 0.91
Std Error Mean = 0.650



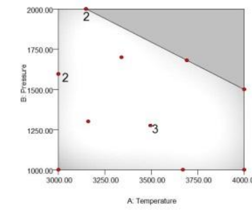
Results*





**(Generated via re-simulation from predictive equations provided in coded form by the experimenters. The graphs closely resemble the published results for the key measures of dynamic pressure (Q) and total sensible enthalpy (Hts).)*

Agenda



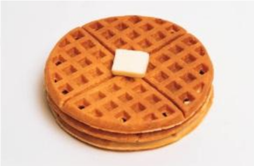
- ✓ What's required for a good design.
- ✓ Optimal point selection (*IV versus D optimality*).
- ✓ Practical aspects algorithmic design.
- ✓ Optimal design example.
- ❑ **Conclusion and recommendations.**

Practical Aspects of DOE

Remember what is Most Important

1. Identify opportunity and define objective.
2. State objective in terms of measurable responses.
   - Define the precision desired to predict each response.
   - Estimate experimental error (σ) for each response.
3. Select the input factors and ranges to study.
4. Select a design and:
   - Evaluate precision via the FDS plot.
   - Examine the design layout to ensure all the factor combinations are safe to run and are likely to result in meaningful information (no disasters).

When Optimal Design is Necessary



- Multiple linear constraints, such waffles made at right temperature and time—not too little (runny!) and not too much (burnt!)
- Factors are categoric or discrete numeric
- Models other than full quadratic handled by cataloged RSM designs such as central composite

Always choose a design that fits the problem!

Size for precision!

Practical Aspects Algorithmic Design

Optimality Criteria

Should I use a D-optimal or IV-optimal design?

- IV-optimal - precise estimation of the predictions
  - Best for empirical response surface design
- D-optimal - precise estimation of model coefficients
  - Best for screening and mechanistic models

Practical Aspects Algorithmic Design

Suggestion for Point Selection

Given how many factors (k) you study and the number of coefficients (p) in the model you select, use the following as a guide to a starting design:

- Model: p points using an optimality criteria
- Lack-of-Fit: 5 points; based on distance or estimating higher order model terms.
- Replicates: 5 points, using the model optimality criteria (most influential).

Evaluate precision of the starting design via the FDS plot:

- If more precision is required, rebuild the design adding more runs.

Practical Aspects of DOE

Keep in Mind

No alphabetic optimality or sophisticated statistical analysis can make up for:

- Studying the wrong problem.
- Measuring the wrong response.
- Not having adequate precision.
- Testing the wrong factors.
- Having too many runs outside the region of operability.

Thank you for your attention!

Practical Aspects for Designing Statistically Optimal Experiments

from an engineer's perspective

Mark Anderson, PE
Stat-Ease, Inc.
mark@statease.com

Pat Whitcomb
Stat-Ease, Inc.