SUPERSATURATED DESIGNS: RESEARCH-BASED BEST PRACTICES AND THE FUTURE

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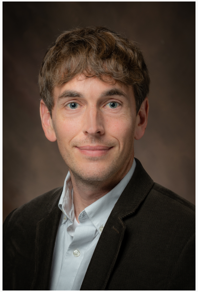

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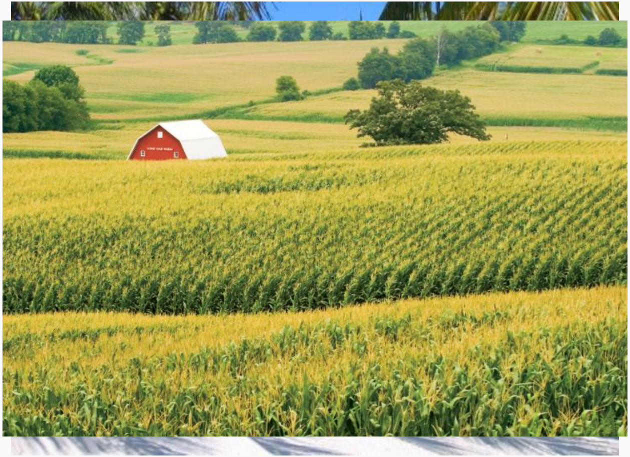


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WHERE ARE THE SUPERSTAURATED DESIGNS?

A quick Google scholar search for “supersaturated design” yields 671 results.

Georgiou, S.D. (2014) provides a review of design construction containing 89 references.

We have found 7 papers containing the results of an experiment using a supersaturated design.

RESEARCH QUESTIONS

Why haven't these designs, which promise such resource-efficiency, been more widely used in industry which so prizes efficiency?

What would it take for supersaturated designs to become a standard tool in the toolkit of experimenters?

What can we, as researchers, do to facilitate the use of SSDs as the first choice for screening?

OUTLINE

1. Informal survey of the design community.
2. Discussion of screening.
3. Practical advice for using supersaturated designs (SSDs).
4. Direction of future research.

SSD DEFINITION

Two-level supersaturated designs (SSDs) use $n < k + 1$ runs to examine k factors. This design uses $n = 6$ runs to examine $k = 9$ factors.

$$D = \begin{pmatrix} -1 & -1 & -1 & 1 & 1 & 1 & 1 & 1 & -1 \\ 1 & 1 & -1 & 1 & 1 & 1 & -1 & -1 & 1 \\ -1 & -1 & 1 & 1 & -1 & -1 & -1 & 1 & 1 \\ 1 & -1 & -1 & 1 & -1 & -1 & 1 & -1 & -1 \\ -1 & 1 & 1 & -1 & -1 & 1 & -1 & -1 & -1 \\ 1 & 1 & -1 & -1 & -1 & 1 & 1 & 1 & 1 \end{pmatrix}$$

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We assume we wish to estimate the model with only linear main effects:

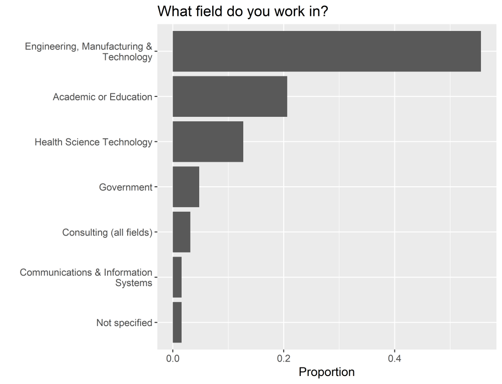
$$Y_i = \beta_0 + \sum_{j=1}^{k} \beta_j x_{ij} + \epsilon_i, \quad i = 1, 2, \ldots, n$$

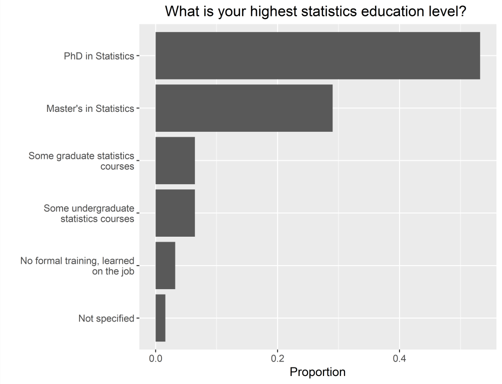
with $\epsilon_i \sim N(0, \sigma^2)$ and are independent.

Informal Survey

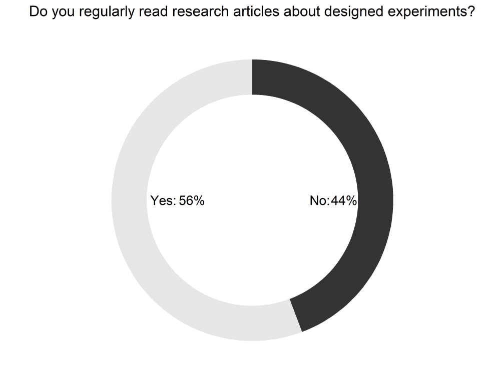
WHO DID WE SURVEY?

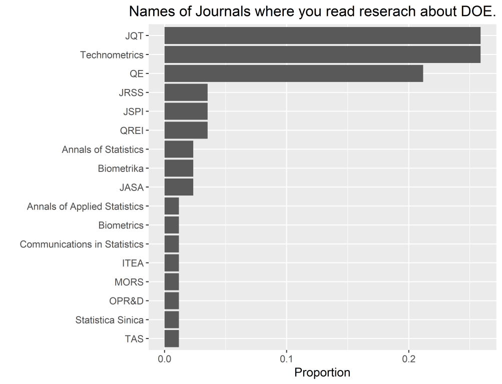
We used our informal networks and social media to reach out to the greater design of experiments community. The following analysis is based on 63 survey responses.



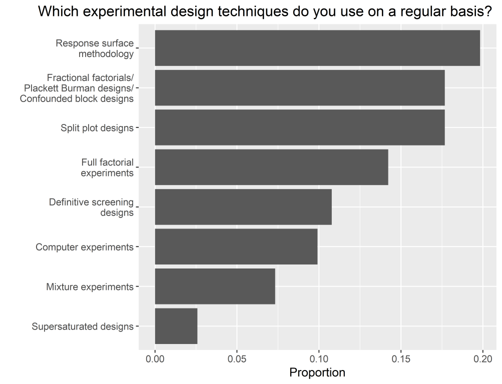


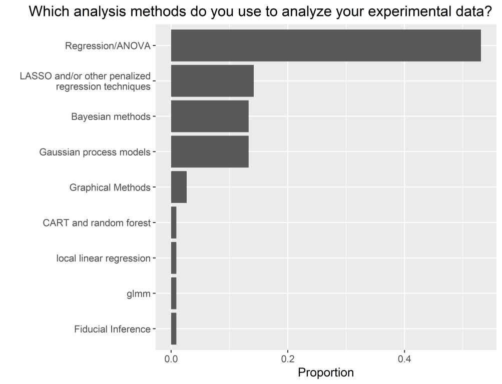
DO YOU READ RESEARCH ABOUT DOE?



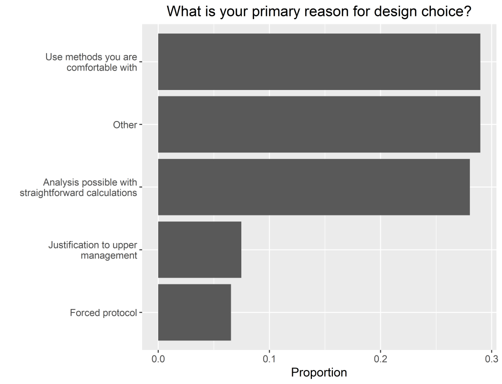


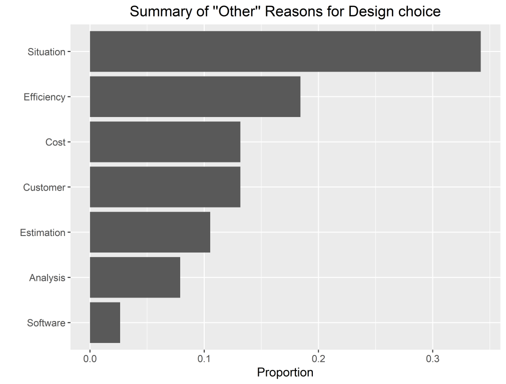
COMMONLY USED DESIGNS AND ANALYSIS METHODS



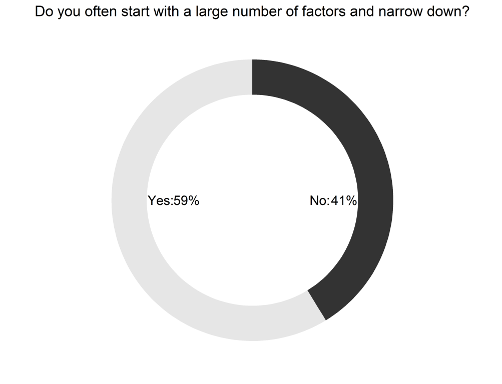


HOW DO PEOPLE DECIDE ON THE DESIGNS THEY USE?





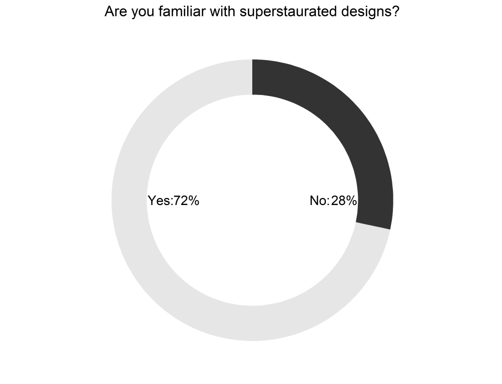
DO YOU REDUCE THE NUMBER OF POSSIBLE FACTORS?

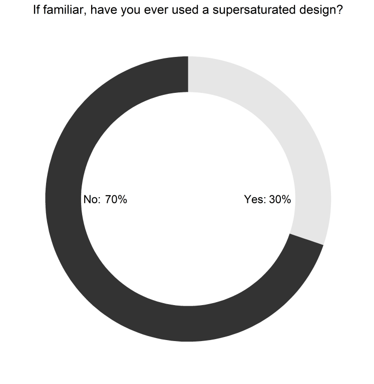


Examples of reduction in factors:

- “75 reduced to 11”
- “Yes. Screen 27, RSM 5.”
- “20 to 5”
- “8-12 down to 6”
- “15, 5”
- “5 down to 3”

WHAT ABOUT SUPERSATURATED DESIGNS?





USER EXPERIENCE WITH SSDS

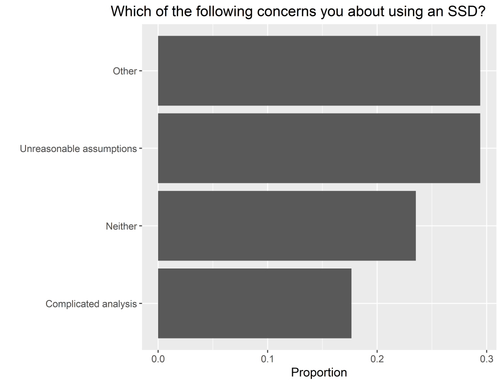
“100+ factors 64 runs; failed experiment”

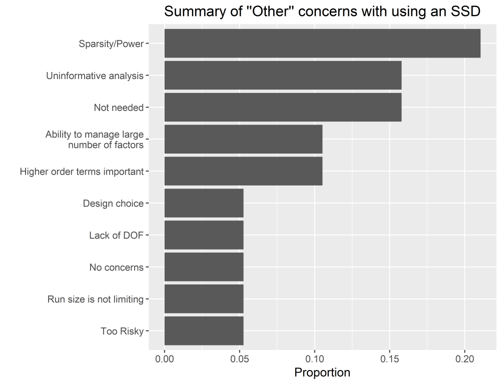
“Bayesian D-optimal design with many terms that were able to be estimated by the design, but were able to be estimated after unimportant factors were removed.”

“Analytical Method Robustness testing. Successful.”

“Testing to characterize drill bit effectiveness as a function of many input parameters. Experiment was successful due to engineering expertise for interpretation.”

CONCERNS WITH USING A SSD





CONTRADICTION IN LITERATURE

"I think it is perfectly natural and wise to do some supersaturated experiments."–John Tukey, 1959

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"We have no experience of practical problems where such designs are likely to be useful; the conditions that interactions should be unimportant and that there should be a few dominant effects seems very severe."–Kathleen Booth and D.R. Cox 1962

CONTRADICTION IN LITERATURE

"'… we can say that one should be very cautious when using any method for constructing, analyzing or generally using SSDs."–Stelios Georgiou 2014

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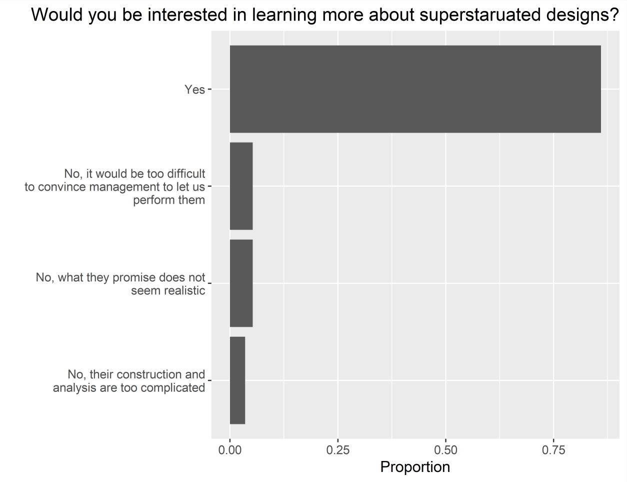
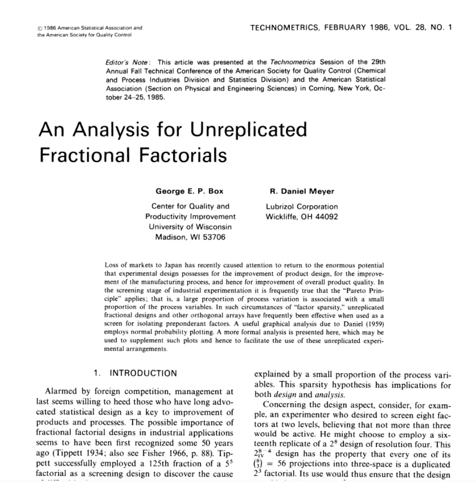
"For situations where there really is no prior knowledge of the effects of factors, but a strong belief in factor sparsity, and where the aim is to find out if there are any dominant factors and to identify them, experimenters should seriously consider using supersaturated designs."–Steven Gilmour 2006

WOULD YOU WANT TO LEARN MORE?



Screening

The success of screening experiments depends heavily on the assumptions of effect sparsity and effect hierarchy.



TECHNOMETRICS, FEBRUARY 1986, VOL. 28, NO. 1

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An Analysis for Unreplicated Fractional Factorials

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Loss of markets to Japan has recently caused attention to return to the enormous potential that experimental design possesses for the improvement of product design, for the improvement of the manufacturing process, and hence for improvement of overall product quality. In the screening stage of industrial experimentation it is frequently true that the "Pareto Principle" applies; that is, a large proportion of process variation is associated with a small proportion of the process variables. In such circumstances of "factor sparsity," unreplicated fractional designs and other orthogonal arrays have frequently been effective when used as a screen for isolating preponderant factors. A useful graphical analysis due to Daniel (1959) employs normal probability plotting. A more formal analysis is presented here, which may be used to supplement such plots and hence to facilitate the use of these unreplicated experimental arrangements.

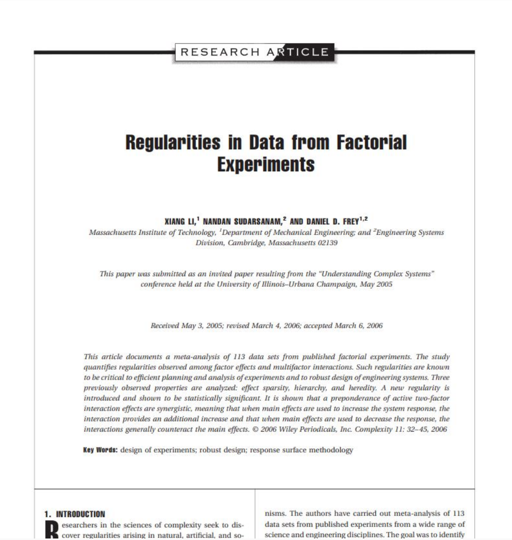
1. INTRODUCTION

Alarmed by foreign competition, management at last seems willing to heed those who have long advocated statistical design as a key to improvement of products and processes. The possible importance of fractional factorial designs in industrial applications seems to have been first recognized some 50 years ago (Tippett 1934; also see Fisher 1966, p. 88). Tippett successfully employed a 125th fraction of a 5^5 factorial as a screening design to discover the cause

explained by a small proportion of the process variables. This sparsity hypothesis has implications for both *design* and *analysis*.

Concerning the design aspect, consider, for example, an experimenter who desired to screen eight factors at two levels, believing that not more than three would be active. He might choose to employ a sixteenth replicate of a 2^8 design of resolution four. This 2^{8-4}_{IV} design has the property that every one of its $\binom{8}{3} = 56$ projections into three-space is a duplicated 2^3 factorial. Its use would thus ensure that the design

These principles have been
empirically verified and quantified.


RESEARCH ARTICLE

Regularities in Data from Factorial Experiments

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This article documents a meta-analysis of 113 data sets from published factorial experiments. The study quantifies regularities observed among factor effects and multifactor interactions. Such regularities are known to be critical to efficient planning and analysis of experiments and to robust design of engineering systems. Three previously observed properties are analyzed: effect sparsity, hierarchy, and heredity. A new regularity is introduced and shown to be statistically significant. It is shown that a preponderance of active two-factor interaction effects are synergistic, meaning that when main effects are used to increase the system response, the interaction provides an additional increase and that when main effects are used to decrease the response, the interactions generally counteract the main effects. © 2006 Wiley Periodicals, Inc. Complexity 11: 32–45, 2006

Key Words: design of experiments; robust design; response surface methodology

1. INTRODUCTION

Researchers in the sciences of complexity seek to discover regularities arising in natural, artificial, and so-

nisms. The authors have carried out meta-analysis of 113 data sets from published experiments from a wide range of science and engineering disciplines. The goal was to identify

TRADITIONAL SCREENING DESIGNS AND ANALYSIS

Traditional screening designs are constructed with good Least Squares estimation properties, such as a "small" covariance matrix, $\sigma^2(\mathbf{X}^\top\mathbf{X})^{-1}$.

"Small" covariance is achieved in classical screening by ensuring a design matrix, $\mathbf{D}$, has orthogonal columns.

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“Small” covariance is achieved in classical screening by ensuring a design matrix, $\mathbf{D}$, has orthogonal columns.

Is this the best strategy for a SSD where $n < k$?

SUCCESSFUL SCREENING DEFINED

The goal of screening is not to make precise estimates, but to identify important factors.

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The screening results would be perfect, but the estimators would be poor.

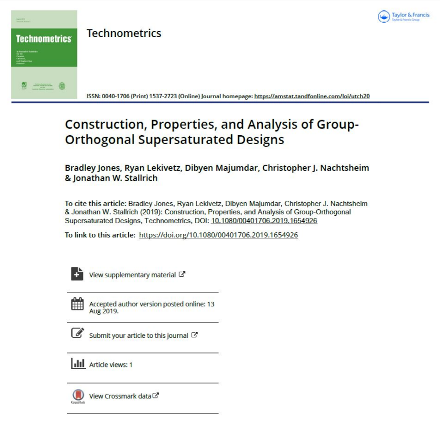
SUCCESSFUL SCREENING DEFINED

To identify the truly important factors as important the SSD/analysis combination must have high power to detect those truly active factors.

In many cases we might consider a screening experiment successful, even high power came at a cost of increased type I error.

SSDs should be constructed to enhance factor identification, not estimation.

Two recent example of SSDs that exploit SSD structure to maximize factor identification are the GO-SSD approach of Jones et al. (2019) and Var(s)+ of Weese et al. (2017)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Construction, Properties, and Analysis of Group-Orthogonal Supersaturated Designs

Bradley Jones, Ryan Lekivetz, Dibyen Majumdar, Christopher J. Nachtsheim & Jonathan W. Stallrich

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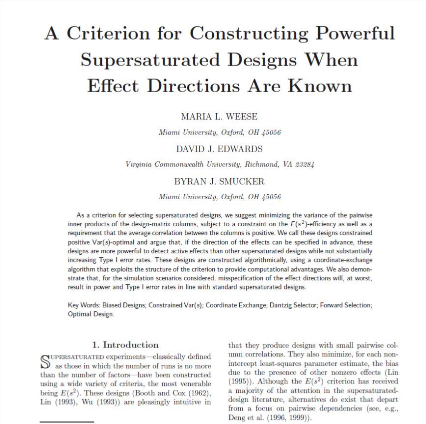
A Criterion for Constructing Powerful Supersaturated Designs When Effect Directions Are Known

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As a criterion for selecting supersaturated designs, we suggest minimizing the variance of the pairwise inner products of the design-matrix columns, subject to a constraint on the $E(s^2)$-efficiency as well as a requirement that the average correlation between the columns is positive. We call these designs constrained positive Var(s)-optimal and argue that, if the direction of the effects can be specified in advance, these designs are more powerful to detect active effects than other supersaturated designs while not substantially increasing Type I error rates. These designs are constructed algorithmically, using a coordinate-exchange algorithm that exploits the structure of the criterion to provide computational advantages. We also demonstrate that, for the simulation scenarios considered, misspecification of the effect directions will, at worst, result in power and Type I error rates in line with standard supersaturated designs.

Key Words: Biased Designs; Constrained Var(s); Coordinate Exchange; Dantzig Selector; Forward Selection; Optimal Design.

1. Introduction

Supersaturated experiments—classically defined as those in which the number of runs is no more than the number of factors—have been constructed using a wide variety of criteria, the most venerable being $E(s^2)$. These designs (Booth and Cox (1962), Lin (1993), Wu (1993)) are pleasingly intuitive in that they produce designs with small pairwise column correlations. They also minimize, for each non-intercept least-squares parameter estimate, the bias due to the presence of other nonzero effects (Lin (1995)). Although the $E(s^2)$ criterion has received a majority of the attention in the supersaturated-design literature, alternatives do exist that depart from a focus on pairwise dependencies (see, e.g., Deng et al. (1996, 1999)).

We will focus on the approach of Weese et al (2017) since it is more flexible than the approach of Jones et al. (2019).

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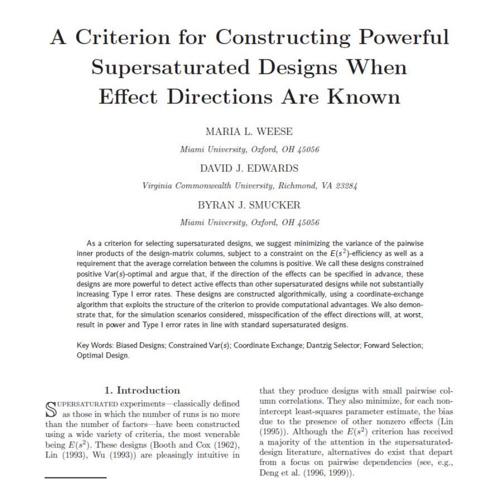
Weese et al. (2017) introduced the Var(s)+ criterion for constructing SSDs to increase power to detect the truly active factors.



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DESIGN CONSTRUCTION: $E(s^2)$ OPTIMALITY

Letting $\mathbf{X} = (\mathbf{1}|\mathbf{D})$ and $\mathbf{S} = \mathbf{X}^T\mathbf{X} = (s_{ij})$ where $i, j = 0, 1, \ldots, k$, we measure a design's proximity to orthogonality by examining the s_{ij}'s, the off-diagonals.

The $E(s^2)$-measure of $\mathbf{X}$ is defined on balanced designs, i.e. those satisfying $\mathbf{1}^T\mathbf{D} = 0$, as

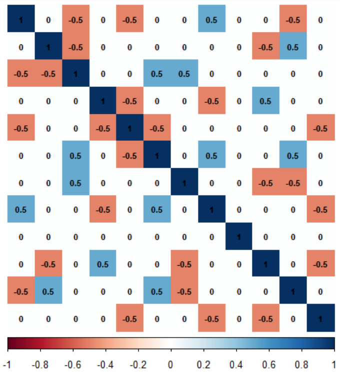
$$\frac{2}{m(m-1)} \sum_{1 \leq i < j \leq m} s_{ij}^2 \ . \tag{1}$$

The $E(s^2)$-criterion minimizes (1) over all balanced designs with n runs and we call such a design $E(s^2)$-optimal.

The constrained Var(s)+ criterion, which we seek to minimize, is:

$$\text{Var}(s)+ = E(s^2) - E(s)^2 \;\; \text{s.t.} \; \frac{E(s^2)(D^*)}{E(s^2)} > c \text{ and } E(s) > 0, \tag{2}$$

where D^* is the $E(s^2)$-optimal design and c is a specified efficiency that determines how near to $E(s^2)$-optimality the design is required to be.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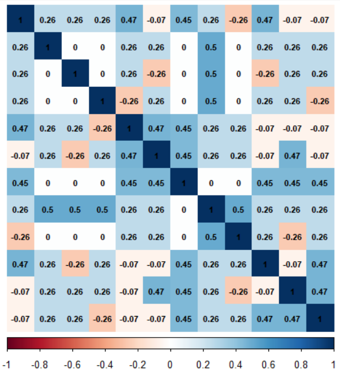
$E(s^2)$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0.26 0 0 1 -0.26 0.26 0 0.5 0 0.26 0.26 -0.26
0.47 0.26 0.26 -0.26 1 0.47 0.45 0.26 0.26 -0.07 -0.07 -0.07
-0.07 0.26 -0.26 0.26 0.47 1 0.45 0.26 0.26 -0.07 0.47 -0.07
0.45 0 0 0 0.45 0.45 1 0 0 0.45 0.45 0.45
0.26 0.5 0.5 0.5 0.26 0.26 0 1 0.5 0.26 0.26 0.26
-0.26 0 0 0 0.26 0.26 0 0.5 1 0.26 -0.26 0.26
0.47 0.26 -0.26 0.26 -0.07 -0.07 0.45 0.26 0.26 1 -0.07 0.47
-0.07 0.26 0.26 0.26 -0.07 0.47 0.45 0.26 -0.26 -0.07 1 0.47
-0.07 0.26 0.26 -0.26 -0.07 -0.07 0.45 0.26 0.26 0.47 0.47 1
-1 -0.8 -0.6 -0.4 -0.2 0 0.2 0.4 0.6 0.8 1

$Var(s)+$

THE DANTZIG SELECTOR

The Dantzig selector (Candes and Tao, 2007), $\hat{\beta}_{\text{DS}}$ imposes a constraint on an ℓ_1-estimator:

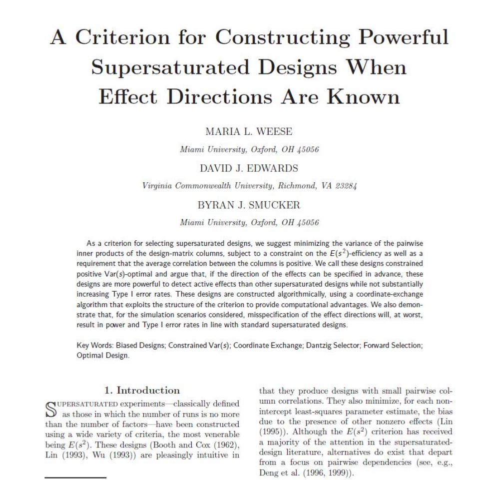
$$\hat{\beta}_{\text{DS}} = \underset{\tilde{\beta}}{\arg\min} \, ||\tilde{\beta}||_1 \text{ subject to } ||X^{\top}(y - X\tilde{\beta})||_{\infty} \leq \delta \,, \tag{3}$$

where $|| \cdot ||_{\infty}$ denotes the largest element of the argument.

$\hat{\beta}_{\text{DS}}$ estimates are biased but still have desirable model selection properties.

VAR(S)+ SSDS+DANTZIG SELECTOR CAN GIVE HIGHER POWER TO DETECT ACTIVE FACTORS

1. If the user can specify the effect directions ahead of time.
2. If the SSD is analyzed using the Dantzig selector.
3. If effect directions are misspecified, the performance is equivalent to existing construction methods.
4. Type I error rate for constrained Var(s)+ designs is not larger



A Criterion for Constructing Powerful Supersaturated Designs When Effect Directions Are Known

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As a criterion for selecting supersaturated designs, we suggest minimizing the variance of the pairwise inner products of the design-matrix columns, subject to a constraint on the $E(s^2)$-efficiency as well as a requirement that the average correlation between the columns is positive. We call these designs constrained positive Var(s)-optimal and argue that, if the direction of the effects can be specified in advance, these designs are more powerful to detect active effects than other supersaturated designs while not substantially increasing Type I error rates. These designs are constructed algorithmically, using a coordinate-exchange algorithm that exploits the structure of the criterion to provide computational advantages. We also demonstrate that, for the simulation scenarios considered, misspecification of the effect directions will, at worst, result in power and Type I error rates in line with standard supersaturated designs.

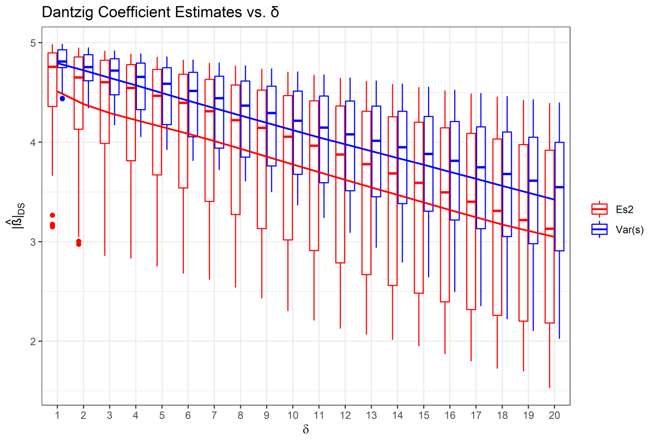
Key Words: Biased Designs; Constrained Var(s); Coordinate Exchange; Dantzig Selector; Forward Selection; Optimal Design.

1. Introduction

Supersaturated experiments—classically defined as those in which the number of runs is no more than the number of factors—have been constructed using a wide variety of criteria, the most venerable being $E(s^2)$. These designs (Booth and Cox (1962), Lin (1993), Wu (1993)) are pleasingly intuitive in that they produce designs with small pairwise column correlations. They also minimize, for each nonintercept least-squares parameter estimate, the bias due to the presence of other nonzero effects (Lin (1995)). Although the $E(s^2)$ criterion has received a majority of the attention in the supersaturated-design literature, alternatives do exist that depart from a focus on pairwise dependencies (see, e.g., Deng et al. (1996, 1999)).

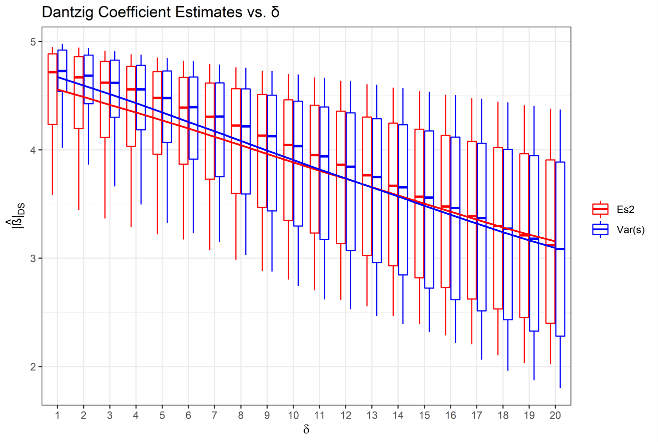
COMPARING DANTZIG ACTIVE COEFFICIENT MAGNITUDES WHEN EFFECT DIRECTION KNOWN

- Generated 1000 responses according to $Y = \beta X + \epsilon$ where $\epsilon \sim N(0, 1)$
- True active coefficients are set to be either all 5 or all -5 (signs are the same)
- Inactive coefficients are set to 0
- Average Dantzig coefficient estimates from Var(s)+ SSDs are larger when effect directions are known



COMPARING DANTZIG ACTIVE COEFFICIENT MAGNITUDES WHEN EFFECT DIRECTION UNKNOWN

- Generated 1000 responses according to $Y = \beta X + \epsilon$ where $\epsilon \sim N(0, 1)$
- True active coefficients are set randomly as 5 or -5 (signs are mixed)
- Inactive coefficients are set to be truly 0
- Average Dantzig coefficient estimates from Var(s)+ SSDs are similar to coefficient estimates from $E(s^2)$ when effect directions are random



Practical Advice for Users

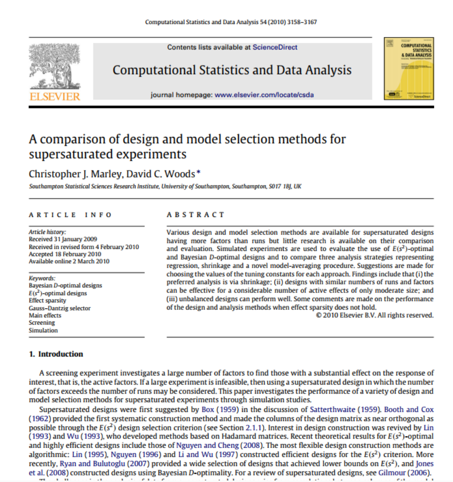
RESEARCH BASED SSD SIZE RECOMMENDATIONS

For a successful experiment using a SSD, Marley and Woods (2010) state the following rules:

1. The ratio of the run size,n, to the number of active factors, a, should be greater than 3.

2. The ratio of the number of factors, k, to n should be no more than 2.

We have replicated these results in separate simulations.



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A comparison of design and model selection methods for supersaturated experiments

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ABSTRACT

Various design and model selection methods are available for supersaturated designs having more factors than runs but little research is available on their comparison and evaluation. Simulated experiments are used to evaluate the use of $E(s^2)$-optimal and Bayesian D-optimal designs and to compare three analysis strategies representing regression, shrinkage and a novel model-averaging procedure. Suggestions are made for choosing the values of the tuning constants for each approach. Findings include that (i) the preferred analysis is via shrinkage; (ii) designs with similar numbers of runs and factors can be effective for a considerable number of active effects of only moderate size; and (iii) unbalanced designs can perform well. Some comments are made on the performance of the design and analysis methods when effect sparsity does not hold.

1. Introduction

A screening experiment investigates a large number of factors to find those with a substantial effect on the response of interest, that is, the active factors. If a large experiment is infeasible, then using a supersaturated design in which the number of factors exceeds the number of runs may be considered. This paper investigates the performance of a variety of design and model selection methods for supersaturated experiments through simulation studies.

Supersaturated designs were first suggested by Box (1959) in the discussion of Satterthwaite (1959). Booth and Cox (1962) provided the first systematic construction method and made the columns of the design matrix as near orthogonal as possible through the $E(s^2)$ design selection criterion (see Section 2.1.1). Interest in design construction was revived by Lin (1993) and Wu (1993), who developed methods based on Hadamard matrices. Recent theoretical results for $E(s^2)$-optimal and highly efficient designs include those of Nguyen and Cheng (2008). The most flexible design construction methods are algorithmic: Lin (1995), Nguyen (1996) and Li and Wu (1997) constructed efficient designs for the $E(s^2)$ criterion. More recently, Ryan and Bulutoglu (2007) provided a wide selection of designs that achieved lower bounds on $E(s^2)$, and Jones et al. (2008) constructed designs using Bayesian D-optimality. For a review of supersaturated designs, see Gilmour (2006).

To use the Dantzig Selector on a SSD in a simulation we use the automated procedure of Phoa et al. (2009) which requires:

1. specification of threshold, γ such that the i^{th} factor is called active if $|\hat{\beta}_\mathrm{i}|_\delta > \gamma$ and
2. a model section statistic to choose the model at some value of δ.

We do not recommend the automated procedure for the analysis of a single experiment.

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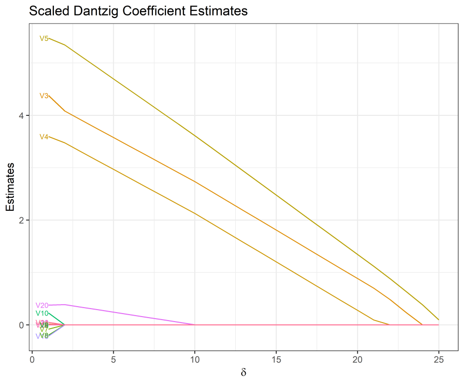
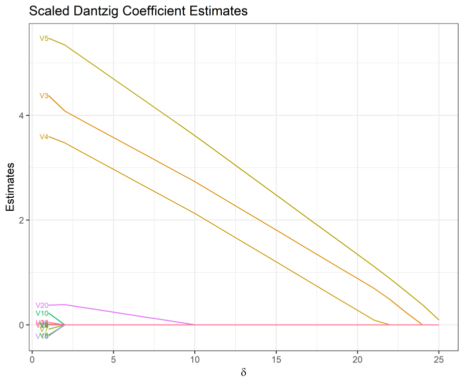
We do not recommend the automated procedure for the analysis of a single experiment.

We also emphasize the importance of centering the response vector, $\mathbf{y}$, and centering and scaling X to unit variance. This is especially important when D is unbalanced since the columns of $\mathbf{D}$ will be correlated with the intercept column in $\mathbf{X}$.

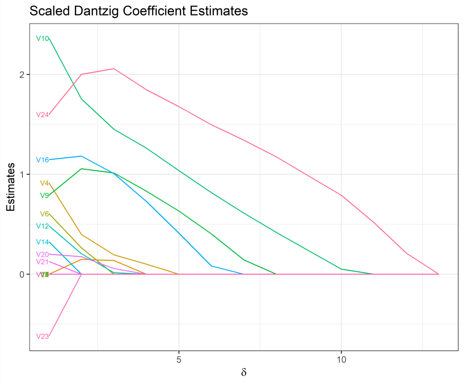
USE A PROFILE PLOT WITH THE DANTZIG SELECTOR



USE A PROFILE PLOT WITH THE DANTZIG SELECTOR



Easy



Not as Easy

The following recommendations help to address the concerns of ”Power/Sparsity” and ”Uninformative Analysis” from the survey respondents:

1. Keep the ratio of factors to runs less than 2.
2. Plan for the number of active effects to be sparse, specifically less than n/3.
3. Specify effect directions ahead of time (even if you have to guess).
4. Construct the SSD using constrained Var(s)+-optimality.
5. Analyze the experiment with the Dantzig Selector using a profile plot making sure to scale properly.

Future Research

NEXT STEPS

1. Investigate smart follow-up experiments for SSD.
2. Inclusion of interactions and higher order terms in a SSD.
3. Further exploit the properties of regularization methods in the structure of new SSDs.

Questions?

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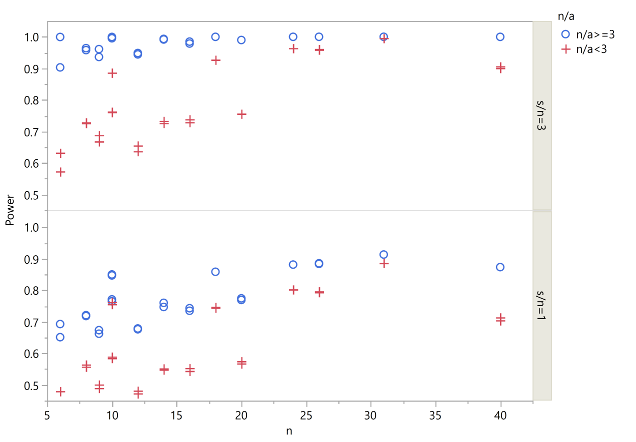
Appendix

NUMBER OF RUNS COMPARED TO THE NUMBER OF ACTIVE FACTORS

- Generated 1000 responses according to $Y = \beta X + \epsilon$ where $\epsilon \sim N(0, 1)$ and $\beta_a \sim \exp(1) + s/n$ where $s/n = 1$ or 3.
- Inactive coefficients are set to 0
- Average Dantzig coefficient estimates from Var(s)+ SSDs are larger when effect directions are known



NUMBER OF FACTORS COMPARED TO THE NUMBER OF RUNS

- Generated 1000 responses according to $Y = \beta X + \epsilon$ where $\epsilon \sim N(0,1)$ and $\beta_a \sim \exp(1) + s/n$ where $s/n = 1$ or 3.
- Inactive coefficients are set to 0
- Average Dantzig coefficient estimates from Var(s)+ SSDs are larger when effect directions are known