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COMPLEXITY IN EXPERIMENTAL DESIGN II. COMPARING SECOND-ORDER DESIGNS

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0. ABSTRACT

Complexity is used together with other criteria to compare eight small second-order designs, with emphasis on the regularity of confidence ellipsoids for the parameters. Similar comparisons are drawn for subsets of parameters consisting of linear, pure quadratic, and interaction coefficients of the model to assess specific design characteristics.

1. INTRODUCTION

Given a model $\mathbf{Y} = \mathbf{f}(\mathbf{X})\boldsymbol{\beta} + \boldsymbol{\varepsilon}$ with design matrix $\mathbf{X}$, the design is often evaluated using estimative criteria such as A, D or E efficiency (cf. Kiefer (1959), Fedorov (1972)) and information functionals (Pukelsheim (1980)), or using predictive criteria such as G efficiency (Kiefer (1959)) and the integrated prediction variance (Box and Draper (1959)). Part I of this study considers complexity (van Emden (1971)) as a further criterion used elsewhere in model selection (Maklad and Nichols (1980)). It is seen that complexity gages the nonorthogonality of $\mathbf{X}$ through the ellipticity of $\boldsymbol{\Sigma} = [\mathbf{f}(\mathbf{X})'\mathbf{f}(\mathbf{X})]^{-1}$, and thereby the degree of regularity of confidence ellipsoids for $\boldsymbol{\beta}$. In particular, complexity is related directly to A-efficiency, and inversely to D-efficiency. In Part II we now apply these concepts in a comparative evaluation of selected second-order designs in current usage.

A partial list includes the central composite designs (*CCD*'s) of Box and Wilson (1951), the small composite designs (*SCD*'s) of Hartley (1959), the designs (*BBD*'s) of Box and Behnken (1960), the minimal designs (*BDD*'s) of Box and Draper (1974), the hybrid designs *H*310 and *H*311*B* of Roquemore (1976), the designs (*HOD*'s) of Hoke (1974), the designs (*NOD*'s) of Notz (1982), and others. Properties of these designs have been reported in the literature.

To fix ideas, consider a second-order model

$$\{Y_i = \beta_0 + \sum_{r=1}^{k} \beta_r X_{ir} + \sum_{r=1}^{k} \beta_{rr} X_{ir}^2 + \sum_{r<s} \beta_{rs} X_{ir} X_{is} + \varepsilon_i;\ i = 1, \dots, n\} \qquad (1.1)$$

in $k = 3$ regressors $\{X_{i1}, X_{i2}, X_{i3}\}$ having $p = 1 + k(k+3)/2 = 10$ parameters given as $\boldsymbol{\beta}' = [\beta_0, \beta_1, \beta_2, \beta_3, \beta_{11}, \beta_{22}, \beta_{33}, \beta_{12}, \beta_{13}, \beta_{23}]$. These are partitioned subsequently as $\boldsymbol{\beta} = [\beta_0, \boldsymbol{\beta}_L', \boldsymbol{\beta}_Q', \boldsymbol{\beta}_I']'$, where $\boldsymbol{\beta}_L' = [\beta_1, \beta_2, \beta_3]$, $\boldsymbol{\beta}_Q' = [\beta_{11}, \beta_{22}, \beta_{33}]$, and $\boldsymbol{\beta}_I' = [\beta_{12}, \beta_{13}, \beta_{23}]$ respectively comprise the linear, the pure quadratic, and the interaction coefficients of the model. We next compare designs for models of this type.

2. COMPARING DESIGNS FOR $\boldsymbol{\beta}$

Of eight designs cited with $k = 3$, all are unsaturated on adding a center run as necessary; all have been scaled to $\sqrt{3}$ at the design perimeter; and the *SCD* and *CCD* have axial points at $\alpha = \sqrt{3} = 1.732$. To compare designs under the model (1.1), let $V(\hat{\boldsymbol{\beta}})/\sigma^2 = \Lambda$ with eigenvalues $\boldsymbol{\lambda} = [\lambda_1, \dots, \lambda_k]'$. The relevant diagnostics are the arithmetic ($\bar{\lambda}$) and geometric ($GM(\boldsymbol{\lambda})$) means of $\boldsymbol{\lambda}$, the complexity coefficient $\phi(\Lambda)$ of van Emden (1971), the ellipticity coefficient $C_0(\Lambda) = (1/k)\mathrm{tr}(\Lambda)/|\Lambda|^{1/k}$, and the trace ($\mathrm{tr}(\Lambda)$) and determinant ($|\Lambda|$) of Λ. The latter determine the *A* and *D* efficiencies for each design, whereas complexity gages regularity of confidence ellipsoids for $\boldsymbol{\beta}$ as noted. However, since $\bar{\lambda} = \mathrm{tr}(\Lambda)/10$, and since $\phi(\Lambda)$ and $C_0(\Lambda)$ are related one-to-one, as are $GM(\boldsymbol{\lambda})$ and $|\Lambda|$, it suffices to report only $C_0(\Lambda)$, $\mathrm{tr}(\Lambda)$, and $20GM(\boldsymbol{\lambda})$ as equivalent gages of complexity (van Emden (1971)) and the *A* and *D* efficiencies for each design. The scaling $20GM(\boldsymbol{\lambda})$ is chosen for convenience. These appear in columns 2 - 4 of Table 1 for each of the eight designs, as they pertain to complexity and efficiency for the full parameters $\boldsymbol{\beta}$.

We prefer $C_0(\Lambda)$ and $GM(\boldsymbol{\lambda})$ to $\phi(\Lambda)$ and $|\Lambda|$. For if designs $\mathbf{X}$ and $\mathbf{Z}$, with $\Sigma = [\mathbf{f}(\mathbf{X})'\mathbf{f}(\mathbf{X})]^{-1}$ and $\Omega = [\mathbf{f}(\mathbf{Z})'\mathbf{f}(\mathbf{Z})]^{-1}$, are of equal complexity, *i.e.,* $C_0(\Sigma) = C_0(\Omega)$, then their comparative *A* and *D* efficiencies are identical as gaged by $C_A(\mathbf{X})/C_A(\mathbf{Z})$ and $C_D(\mathbf{X})/C_D(\mathbf{Z})$, with $C_A(\mathbf{X}) = \mathrm{tr}(\Sigma)$ and $C_D(\mathbf{X}) = |\Sigma|^{1/k}$, and similarly for $C_A(\mathbf{Z})$ and $C_D(\mathbf{Z})$.

From Table 1 designs *BBD* and *CCD* stand out for their greater *A* and *D* efficiencies in comparison with other designs. Designs *H*310 and *CCD* have comparable *A*-efficiencies, but their complexities and *D*-efficiencies are related inversely as shown in Theorem 1 of Part I. The designs *NOD*, *HOD*, and *BDD* are less *A* and *D* efficient than the remaining designs, although their complexities are roughly comparable. Further such comparisons are supported by Table 1, and a summary is provided in Section 4.

3. COMPARISONS FOR SUBSETS OF PARAMETERS

3.1 Background. Special features of a response surface are often germane. Linear coefficients determine slopes at the origin, whereas second-order coefficients determine the shapes and orientations of its contours. Moreover, the signs and magnitudes of interaction coefficients quantify the presence and degree of synergistic or antagonistic effects between pairs of variables, as in studies of the efficacy of drugs in combination. For further discussion see Heady (1952), Heady and Dillon (1961), Myers (1971), Wardrop and Myers (1990), and Myers and Montgomery (1995), for example. Since different uses entail different features, it is essential to compare designs on these issues.

These needs embody the concept of local design efficiencies for subsets of parameters, including A_S, D_S, G_S, and other local criteria as in Atwood (1969), Kiefer (1961), Sibson (1974), and Wardrop and Myers (1990), for example. Here we add local complexity to that list, and we accordingly compare these designs with reference to $\boldsymbol{\beta}_L$, $\boldsymbol{\beta}_Q$, and $\boldsymbol{\beta}_I$ along the lines of the comparisons for $\boldsymbol{\beta}$ as given in Table 1.

3.2 Linear Coefficients. Diagnostics for the linear coefficients $\boldsymbol{\beta}_L$ are reported in the last three columns of Table 1. The designs $\{SCD, HOD, BDD\}$ are comparatively inefficient for $\boldsymbol{\beta}_L$ under both A_S and D_S efficiencies. The HOD has complexity of 1.25, in comparison with the value 1.00 for the other designs. Confidence ellipsoids for $\boldsymbol{\beta}_L$ for the latter designs are all spherical owing to regularity of the designs.

3.3 Quadratic Coefficients. Diagnostics for the pure quadratic coefficients $\boldsymbol{\beta}_Q$ are reported in the first four columns of Table 2. The designs $\{NOD, HOD, BDD\}$ are especially A_S and D_S inefficient for $\boldsymbol{\beta}_Q$. Moreover, all designs have complexities greater than 1. Further trends are summarized in Section 4.

3.4 Interaction Coefficients. Diagnostics for the interaction coefficients $\boldsymbol{\beta}_I$ appear in the last three columns of Table 2. The SCD is especially D_S-inefficient and somewhat A_S-inefficient, followed by BDD, $H311B$, and HOD. In practice these would be avoided in studies of synergism and antagonism, in favor of designs $\{BBD, CCD, NOD\}$. The HOD has complexity of 1.24, in comparison with values at or near 1.00 for the other designs. Further trends are summarized in the section following.

4. CONCLUSIONS

A recurring problem is to choose among the many second-order designs now available using appropriate criteria. The approach taken here features the regularity of confidence ellipsoids for the parameters, placing yet another tool in the hands of prospective users. A summary of our findings follows, where the grouping and ordering $\{D_1, D_2\} \succ \{D_3\}$ is meant to convey the idea that designs D_1 and D_2 are roughly comparable, each being more efficient than design D_3. Regarding complexity, $\{D_1\} \prec \{D_2, D_3\}$ conveys that D_1 is less complex than D_2 and D_3, which are roughly comparable in complexity. With these conventions we may summarize our principal findings as follows.

Efficiencies and complexities for the full parameters $\boldsymbol{\beta}$ satisfy

- A-efficiency: $\{H310, H311B, SCD, BBD, CCD\} \succ \{NOD, HOD, BDD\}$.
- D-efficiency: $\{BBD, CCD\} \succ \{H310, H311B, SCD\} \succ \{NOD, HOD, BDD\}$.
- Complexity: $\{H310, BDD\} \prec \{H311B, BBD, HOD\} \prec \{SCD, CCD, NOD\}$.

Efficiencies and complexities for the linear coefficients $\boldsymbol{\beta}_L$ satisfy

- A_S-efficiency: $\{BBD, CCD\} \succ \{H310, H311B, NOD\} \succ \{SCD, HOD, BDD\}$.
- D_S-efficiency: $\{BBD, CCD\} \succ \{H310, H311B, NOD\} \succ \{SCD, HOD, BDD\}$.
- Complexity: All designs have $C_0(\Lambda) = 1.00$ except HOD with $C_0(\Lambda) = 1.22$.

Efficiencies and complexities for the pure quadratic coefficients $\boldsymbol{\beta}_Q$ satisfy

- A_S-efficiency: $\{H310, H311B, SCD, BBD, CCD\} \succ \{NOD, HOD, BDD\}$.
- D_S-efficiency: $\{H311B, SCD, CCD\} \succ \{H310, BBD\} \succ \{NOD, HOD, BDD\}$.
- Complexity: $\{H310, BDD\} \prec \{BBD, NOD, HOD\} \prec \{H311B, SCD, CCD\}$.

Efficiencies and complexities for the interaction coefficients $\boldsymbol{\beta}_I$ satisfy

- A_S-efficiency: $\{H310, H311B, BBD, CCD, NOD\} \succ \{SCD, HOD, BDD\}$.
- D_S-efficiency: $\{BBD, CCD, NOD\} \succ \{H310, H311B, HOD, BDD\} \succ \{SCD\}$.
- Complexity: All designs have $C_0(\Lambda)$ near 1.00 except HOD with $C_0(\Lambda) = 1.24$.

In summary, a synthesis of our findings suggests that the designs may be grouped as $\{H310, H311B, BBD, CCD\} \succ \{SCD, NOD, HOD, BDD\}$ in terms of overall efficiency. Comparisons of their complexities are less clear, except that designs $H310$ and BDD appear least complex overall in comparison with the other designs.

REFERENCES

Atwood, C. L. (1969). "Optimal and efficient design of experiments." *Ann. Math. Statist.* **40:** 1570-1602.

Box, G. E. P. and Behnken, D. W. (1960). "Some new three-level designs for the study of quantitative variables." *Technometrics* **2:** 455-475.

Box, G. E. P. and Draper, N. R. (1959). "A basis for the selection of a response surface design." *Journal of the American Statistical Association* **54:** 622-654.

Box, G. E. P. and Wilson, K. B. (1951). "On the experimental attainment of optimum conditions." *Journal of the Royal Statistical Society, Series B* **13**: 1-45.

Box, M. J. and Draper, N. R. (1974). "On minimum-point second order designs." *Technometrics* **16**: 613-616.

Emden, M. H. van (1971). "An analysis of complexity." *Mathematical Centre Tracts,* Volume 35. Mathematical Centrum, Amsterdam.

Fedorov, V. V. (1972). *Theory of Optimal Experiments.* Academic Press, New York.

Hartley, H. O. (1959). "Smallest composite design for quadratic response surfaces." *Biometrics* **15**: 611-624.

Heady, E. O. (1952). *Economics of Agricultural Production and Resource Use.* Prentice-Hall, New York.

Heady, E. O. and Dillon, J. L. (1961). *Agricultural Production Functions.* Iowa State University Press, Ames, Iowa.

Hoke, A. T. (1974). "Economical second-order designs based on irregular fractions of the 3^n factorial." *Technometrics* **17**: 375-384.

Kiefer, J. (1959). "Optimum experimental designs." *Journal of the Royal Statistical Society, Series B* **21**: 272-319.

Kiefer, J. (1961). "Optimal design in regression problems, II." *Ann. Math. Statist.* **32**: 298-325.

Maklad, M. S. and Nichols, S. T. (1980). "A new approach to model structure discrimination." *IEEE Transactions on System, Man, and Cybernetics* **10**: 78-84.

Myers, R. H. (1971). *Response Surface Methodology.* Allyn and Bacon, Boston.

Myers, R. H. and Montgomery, D. C. (1995). *Response Surface Methodology: Process and Product Optimization Using Designed Experiments.* John Wiley and Sons, New York.

Notz, W. (1982). "Minimal point second order designs." *Journal of Statistical Planning and Inference* **6**: 47-58.

Pukelsheim, F. (1980). "On linear regression designs which maximize information." *Journal of Statistical Planning and Inference* **4**: 339-364.

Roquemore, K. G. (1976). "Hybrid designs for quadratic response surfaces." *Technometrics* **18**: 419-423.

Sibson, R. (1974). "D_A-optimality and duality." In *Progress in Statistics, Proc. 9th European Meeting of Statisticians, Budapest, 1972, Vol. 2,* J. Gani, K. Sarkadi and I. Vincze, eds., North-Holland, Amsterdam.

Wardrop, D. and Myers, R. H. (1990). "Some response surface designs for finding optimal conditions." *J. Stat. Planning and Inference* **25**: 7-28.

TABLE 1. Diagnostics based on dispersion matrices $V(\hat{\beta})/\sigma^2$ for the full parameters and $V(\hat{\beta}_L)/\sigma^2$ for the linear coefficients of eight small designs.

	Coefficients β			Coefficients β_L		
Design	$C_0(\Lambda)$	tr (Λ)	$20GM(\lambda)$	$C_0(\Lambda)$	tr (Λ)	$20GM(\lambda)$
*H*310	1.3256	1.9873	2.9983	1.0000	0.3565	2.3764
*H*311*B*	1.8743	2.4000	2.5610	1.0000	0.3000	2.0000
SCD	2.0976	3.2278	3.0775	1.0000	0.5000	3.3333
BBD	1.9602	2.1667	2.2107	1.0000	0.2500	1.6667
CCD	2.1953	2.0575	1.8745	1.0000	0.2144	1.4286
NOD	2.0930	4.2500	4.0613	1.0000	0.3750	2.5000
HOD	1.8873	4.4023	4.6652	1.2157	0.6973	3.8238
BDD	1.4383	3.1906	4.4367	1.0000	0.4764	3.1762

TABLE 2. Diagnostics based on dispersion matrices $V(\hat{\beta}_Q)/\sigma^2$ for the quadratic coefficients and $V(\hat{\beta}_I)/\sigma^2$ for the interaction coefficients of eight small designs.

	Coefficients β_Q			Coefficients β_I		
Design	$C_0(\Lambda)$	tr (Λ)	$20GM(\lambda)$	$C_0(\Lambda)$	tr (Λ)	$20GM(\lambda)$
*H*310	1.0302	0.6429	4.1605	1.0000	0.4831	3.2209
*H*311*B*	1.4163	0.5000	2.3536	1.0000	0.6000	3.9999
SCD	1.5283	0.4778	2.0842	1.0000	1.2500	8.3333
BBD	1.1814	0.5833	3.2917	1.0000	0.3333	2.2222
CCD	1.5110	0.4683	2.0660	1.0000	0.3750	2.5000
NOD	1.1218	2.6250	15.6006	1.0000	0.3750	2.5000
HOD	1.2493	2.4785	13.2263	1.2402	0.7266	3.9055
BDD	1.0546	1.5712	9.9325	1.0012	0.6781	4.5150