White paper on optimal design tools

By Mark J. Anderson (Prepared in January 2009 as a briefing for Stat-Ease, Inc.) – *Revised 12/29/10*

Executive summary

1. Our new version of Design-Expert now offers additional optimal design options – not just D-optimal. The most popular of these new options is likely to be the "IV" optimal design, which makes use of an integrated variance criterion that minimizes the average variance for responses throughout a region of interest. An IV-optimal design tends to place fewer runs at the extremes of the experimental region than D-optimal.
2. The "IV" optimal designs by Stat-Ease are equivalent to the "I" optimal capability of JMP.
3. JMP's "I" optimal really should be called "V" optimal, because they do not minimize the mean squared prediction error (MSPE) as called for by the "I" criterion (see Wikipedia entry below).

Advice from Pat Whitcomb (re 12/27/10 StatHelp question about E-optimality)

I-optimal (or IV-optimal) designs minimize the integral of the prediction variance across the design space. When the goal is prediction (usually the case with empirical response surface designs), I clearly prefer IV-optimal designs.

E-optimal designs focus on parameter estimation; as do A and D optimal designs. In terms of the joint confidence ellipsoid; A-optimality minimizes the sum of the squares of its axes; E-optimality minimizes the squared length of the major axis; and D-optimality minimizes the volume of the ellipsoid. Of the three, I favor D-optimality because it focuses on reducing the variance of the function, rather than focusing on individual components of the function.

What SAS JMP says

From software brochure at http://www.jmp.com/software/pdf/103044_doe.pdf (some parts underlined by MJA for emphasis)

D-Optimal designs are most appropriate for screening experiments because the optimality criterion focuses on precise estimates of the coefficients. If an experimenter has precise estimates of the factor effects, then it is easy to tell which factors' effects are important and which are negligible. So, D-Optimal designs are most efficient for designing experiments where the primary goal is inference.

I-Optimal designs <u>minimize the average prediction variance</u> inside the region of the factors. This makes I-Optimal designs useful for prediction. As a result, <u>I-optimality is the recommended criterion for JMP response surface designs</u>.

An I-Optimal design tends to place fewer runs at the extremes of the design space than does a D-Optimal design. As a result, D-Optimal designs often predict better at the extreme values of the factors.

NIST/Sematech "Engineering Statistics Handbook"

http://www.itl.nist.gov/div898/handbook/pri/section5/pri52.htm

D-Optimality One popular criterion is D-optimality, which seeks to maximize |X'X|, the determinant of the information matrix X'X of the design. This criterion results in minimizing the generalized variance of the parameter estimates based on a pre-specified model.

A-Optimality Another criterion is A-optimality, which seeks to minimize the trace of the inverse of the information matrix. This criterion results in minimizing the average variance of the parameter estimates based on a pre-specified model.

G-Optimality A third criterion is G-optimality, which seeks to minimize the maximum prediction variance, i.e., minimize max. [d=x'(X'X)-1x], over a specified set of design points.

V-Optimality A fourth criterion is V-optimality, which seeks to minimize the average prediction variance over a specified set of design points.

Wikipedia "Optimal design"

http://en.wikipedia.org/wiki/Optimal_design

A-optimality: One criterion is A-optimality, which seeks to minimize the trace of the inverse of the information matrix. This criterion results in minimizing the average variance of the estimates of the regression coefficients.

D-optimality: A popular criterion is D-optimality, which seeks to maximize |X'X|, the determinant of the information matrix X'X of the design. This criterion results in maximizing the differential Shannon information content of the parameter estimates.

E-optimality: A lesser known design is E-optimality, which maximizes the minimum eigenvalue of the information matrix.

G-optimality: Several designs are concerned with prediction variance. Among these, a popular criterion is G-optimality, which seeks to minimize the maximum entry in the diagonal of the hat matrix X(X'X)-1X'. This has the effect of minimizing the maximum variance of the predicted values.

I-optimality: A second criterion on prediction variance is I-optimality, which seeks to minimize the mean squared prediction error.

V-optimality: A third criterion on prediction variance is V-optimality, which seeks to minimize the average prediction variance.

Ed Vawter blog on "Misuse of the Term "optimized" or optimal" Conditions in the Chemical Literature"

http://www.qdinformation.com/qdisblog/2006/06/13/misuse-of-the-term-optimized-or-optimal-conditions-in-the-chemical-literature/

A **D-optimal design** will give you the best value for each of the b's. This is good in cases where you may be studying eight or ten factors and you want to know the critical process parameters; say the three most important. They do not necessarily give the best results for the prediction of the result.

I-optimal designs however, are generated such that the best possible prediction of the result is what is of interest. It may not be entirely obvious but these are indeed different. Sometimes they may be the same but that is not necessarily the case.

Also see Vawter's white paper on BETTER DESIGNS FOR OPTIMIZATION OF ORGANIC PROCESSES at http://www.qdinformation.com/downloads/Better%20designs.pdf.