Factorwise variance dispersion graphs

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\section*{ABSTRACT}
In this paper, new plots, called factorwise variance dispersion graphs (FVDGs) with accompanying coordinate trace plots (CTPs), are introduced. FVDGs display prediction variances throughout the design space across the levels of each design factor, while CTPs plot the coordinates associated with minimum and maximum prediction variances, and hence $G$-efficiencies. FVDGs and CTPs can supplement the use of other graphical tools (e.g., variance dispersion graphs and fraction of design space plots) when assessing the prediction variance properties of a response surface design. They also can be used to assess the robustness of designs with respect to model reduction, design augmentation, and with an irregular design space as in a mixture experiment. Examples and the benefits of FVDGs and CTPs will be presented.

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\section*{1. Introduction}
Consider the experimental situation of having to select a response surface (RS) design having $k$ factors. The problem of choosing a “best” RS design for fitting the parameters of a linear model depends on the criterion of choice. For example, the experimenter could want a design that will produce RS model coefficient estimates with smallest variance or instead could want an orthogonal design. For second or higher-order polynomial RS models, there is not a unique class of “best” designs (Box and Hunter 1957), and it is recommended that coefficient estimates should be studied simultaneously. Therefore, one desirable RS design property is to produce predicted values with small variance.

To address this issue, graphical methods for evaluating prediction variance properties throughout the experimental region have been developed to supplement the use of single-value design optimality criteria, such as $D$ and $G$ optimality (Atkinson et al. 2007). One method is the variance dispersion graph (VDG). VDGs are plots of the minimum, maximum, and average scaled prediction variances (SPVs) in relation to a distance from the center of the design space, and were introduced in Giovannitti-Jensen and Myers (1989) followed by Myers et al. (1992). Vining (1993) provided a Fortran program that generates VDGs with a table of coordinates for the minimum and maximum SPVs. Trinca and Gilmour (1998, 1999) used VDGs to compare prediction variances of RS designs with and without orthogonal blocking and developed the difference variance dispersion graph
(DVDG) for use when the differences in experimental responses are being studied, and also when blocking is used. Liang et al. (2006) used three-dimensional VDGs to study the prediction variance in experiments with a split-plot structure due to hard-to-change factors. Nguyen and Borkowski (2008) introduced a modification of VDGs (called prediction variance volatility (PVV) plots) which augment a VDG with the inclusion of a large number of randomly-generated points in the design space.

Another graphical method is the fraction of design space (FDS) plot which was introduced by Zahran et al. (2003). An FDS plot involves plotting the quantiles of the SPV in relation to the volume of the design region. Ozol-Godfrey et al. (2005) used FDS plots to examine model robustness that allowed comparison of designs across a set of potential models. Park et al. (2005) used both VDGs and FDS plots to compare SPV properties of various designs in cuboidal regions. Rodriguez-Sifuentes et al. (2012) used FDS plots to study prediction variance properties of combined array designs with control and noise variables. Liang et al. (2006) used FDS plots to study the prediction variance in experiments with a split-plot structure due to hard-to-change factors. Ozol-Godfrey et al. (2008) extended the use of FDS plots to study robustness to model misspecification in generalized linear models. Li et al. (2009) studied the prediction variance of large central composite design using SPV plots. Anderson-Cook et al. (2009) used FDS plots to study the prediction variance under potential model misspecification. They also included plots of expected squared bias and expected mean squared error.

For experiments with mixtures having constraints on the component proportions, the mixture design space becomes an irregularly-shaped polyhedron contained in a simplex. Piepel and Anderson (1993) developed plots that display properties of the prediction variance on shrunken polyhedral spaces while Vining, Cornell, and Myers (1993) developed the prediction variance trace in which the prediction variance is plotted in each Cox-effect direction (Cox, 1971). Goldfarb et al. (2004) introduced three-dimensional VDGs for Mixture-Process Experiments to study the prediction variance mixture-process variable designs. Borkowski (2006) introduced componentwise variance dispersion graphs (CVDGs) for mixture experiments in which the minimum, maximum, and average scaled predictions are plotted across the set of feasible component levels for each mixture component.

The graphical concepts behind CVDGs for mixture experiments will be generalized to response surface designs in cuboidal and spherical design spaces. In addition, the PVV plotting method, which was not used with CVDGs, will now be incorporated to create new plots called factorwise variance dispersion graphs (FVDGs). FVDGs are a set of plots of the scaled prediction variance (or, sometimes the prediction variance) throughout the entire design space. FVDGs supplement the use of variance dispersion graphs (VDGs) and fraction of design space (FDS) plots when assessing the prediction variance properties of a response surface design throughout the design space.

In this paper, a brief review of VDGs, FDS plots, PVV plots, and CVDGs will be given. Then FVDGs and modified CVDGs will be defined with examples given for designs in cuboidal, spherical, and mixture design spaces.

1.1. Variance dispersion graphs (VDGs)

Consider a $k$-factor response surface (RS) experiment having $N$ experimental runs. The design matrix $D$ is the $N \times k$ matrix whose rows correspond to factor settings for
the $N$ experimental runs. For any $p$-parameter polynomial RS model, $D$ is expanded to form the $N \times p$ model matrix $X$ with columns corresponding to the $p$ terms in the model.

Assuming IID errors with variance $\sigma^2$, the prediction variance at a point $x$ in the experimental design region is $\text{var}(\hat{Y}(x)) = \sigma^2 V_1(x)$ where $V_1(x) = x_m'(X'X)^{-1}x_m$ and column vector $x_m$ is the RS model expansion of $x$. The scaled prediction variance (SPV) function $V(x)$ is defined as

$$V(x) = \frac{N}{\sigma^2} \text{var}(\hat{Y}(x)) = NV_1(x). \quad (1)$$

For VDGs, three properties of interest involve the scaled prediction variance (SPV) function $V(x)$ in (1). The first property is the average spherical prediction variance $V_\rho$ which is the expected value of $V(x)$ on the surface of the sphere $S_\rho$ of radius $\rho$ from the origin:

$$V_\rho = \frac{1}{\omega_\rho} \int_{S_\rho} N x_m'(X'X)^{-1} x_m \ d x \quad (2)$$

where $\omega_\rho$ is the surface area of $S_\rho$. The other two properties are the minimum and maximum spherical prediction variances given radius $\rho$:

$$V_{\text{MIN}} = \min_{x \in S_\rho} V(x) \quad \text{and} \quad V_{\text{MAX}} = \max_{x \in S_\rho} V(x). \quad (3)$$

To compare the prediction variance properties of RS designs, $V_\rho$, $V_{\text{MIN}}$, and $V_{\text{MAX}}$ are plotted against $\rho$ generating variance dispersion graphs or VDGs. The $V_{\text{MIN}}$ and $V_{\text{MAX}}$ plots provide information regarding the relative stability of $V(x)$ throughout a spherical design space. A horizontal line at $V(x) = p$ (the number of model parameters) is included because $p$ is the optimal value of $V_{\text{MAX}}$ in the design space.

Figure 1 contains VDGs of $V_\rho$, $V_{\text{MIN}}$, and $V_{\text{MAX}}$ for two 3-factor 16-point designs in a spherical design space: the Box-Behnken design (BBD) having 4 center points and the central composite design (CCD) having 2 center points (see Figure 1). To generate the VDG for the BBD, the design points have been scaled by $\sqrt{3}/2$ so that non-center points lie on the surface of a sphere of radius $\sqrt{3}$ (like the points of the CCD). Note that no data is collected in the BBD at the 8 vertices of the cube $(\pm 1, \pm 1, \pm 1)$ which have radii $= \sqrt{3}$. Therefore, the $V_{\text{MAX}}$ curve increases rapidly as $\rho \to \sqrt{3}$. This is not the case for the CCD which contains the eight vertices as well as 6 axial points having radius $\sqrt{3}$. Thus, the $V_{\text{MAX}}$ curve for the CCD remains small and close to the $V_{\text{MIN}}$ curve as $\rho \to \sqrt{3}$.

1.2. Prediction variance volatility (PVV) plots

A prediction variance volatility (PVV) plot is a modification of a VDG (Nguyen and Borkowski 2008). In a PVV plot, $V(x)$ is calculated for a large number of randomly-generated points in the design space $\mathcal{R}$ and these $V(x)$ values are then superimposed on VDGs.
Figure 2 contains PVV plots for 5-factor and 6-factor Box-Behnken designs (BBDs). In each PVV plot, the SPVs for 10000 randomly-generated points are plotted against the associated $q$ values. For the 5-factor BBD, the points are concentrated near $V_{max}$ for all $q$ with very low concentrations near $V_{min}$. However, for the 6-factor BBD, the points...
are concentrated midway between \( V_{\text{min}} \) and \( V_{\text{max}} \) for all \( \rho \). These PVV plots show the “volatility” of the scaled prediction variances. Nguyen and Borkowski (2008) also showed that PVV plots are useful for studying rotatability properties of a design. That is, for designs approaching near-rotatable, the PVV plot becomes less volatile. That is, \( V_{\text{min}} \) is close to \( V_{\text{max}} \) with the PPV plot being a single curve for a rotatable design.

1.3. Fraction of design space (FDS) plots

For a response surface design, it is common to have regions with small \( V(x) \) values while other regions having large \( V(x) \) values. Therefore, it would be useful to assess the prediction variance properties of a design throughout the entire design space \( \mathcal{R} \). Although VDGs and PVV plots show the maximum and minimum values of \( V(x) \) for a given \( \rho \), the information provided in these plots visually assign the same weight at each \( \rho \). That is, they do not provide any information relating \( \rho \) to the volume of the design region. Thus, it is reasonable for the prediction variances to be weighted by the proportion of the design region.

The proportion of a spherical design region accounted for by all points within radius \( \rho \) of the design center is a quadratically increasing function of \( \rho \). As the number of design factors increases, the proportion of the design region becomes negligible for \( \rho \) close to zero but increases rapidly as \( \rho \) increases. Zahran et al. (2003) proposed the fraction of design space or FDS plot which involves plotting the quantiles \( Q \) of \( V(x) \) against \( P \), the proportion of the volume of the design region \( \mathcal{R} \) for which \( V(x) \leq Q \) for any specified value \( Q \). Thus, an FDS plot is essentially a cumulative distribution plot (CDF) of the SPV values in the design region but with the plotting axes reversed in a CDF plot. Figure 3 contains the FDS plots for the two 16-point BBD and CCD plots shown in Figure 1. Note that the quantiles for the first half of the distribution of SPV values for the BBD are smaller than those for the CCD. However, after the median, the CCD quantiles are smaller than those for the BBD with large differences as the FDS \( \rightarrow 1 \).

![Figure 3. FDS Plots for 16-Point BBD (-- --) and CCD with \( z = \sqrt{3} \) (- - - - - -).](image-url)
2. Factorwise variance dispersion graphs (FVDGs)

A new graphical tool called the factorwise variance dispersion graph (FVDG) will be presented. A FVDG is a generalization of CVDGs (Borkowski 2006) in which modified VDG and PVV plots are generated for each factor in the experiment.

To generate a FVDG for the $i^{th}$ design factor ($i = 1, 2, \ldots, k$), fix the factor level $x_i = a$ subject to $L_i \leq a \leq U_i$ where $L_i$ and $U_i$ are the minimum and maximum coded levels considered for $x_i$ in the design space $\mathcal{R}$. For example, if the design space is a hypercube, then $L_i = -1$ and $U_i = +1$, or if the design space is a hypersphere of radius $\sqrt{k}$, then $L_i = -\sqrt{k}$ and $U_i = +\sqrt{k}$.

Let $V(x|x_i = a), VMIN(x|x_i = a)$, and $VMAX(x|x_i = a)$ be the average, minimum, and maximum of $V(x)$ conditioned on $x_i = a$ for all design points $x \in \mathcal{R}$. The following steps outline the procedure for generating a FVDG for one design factor. These two steps would be performed for each design factor $x_i$ for $i = 1, 2, \ldots, k$ producing a set of $k$ FVDGs.

1. For factor $x_i$, plot $V(x|x_i = a), VMIN(x|x_i = a)$, and $VMAX(x|x_i = a)$ curves across the set of $x_i = a$ values such that $L_i \leq a \leq U_i$.
2. Calculate $V(x)$ for a large number of randomly-generated points in $\mathcal{R}$. Superimpose these points to the plot from Step 1.
3. (Optional) Generate a coordinate trace plot (CTP) associated with $VMIN_\rho$ and $VMAX_\rho$ for each $x_i$. For example, the coordinate trace for $x_1$ will have $x_1$ on the horizontal axis. The levels (or coordinates) of the other $x_i$ that correspond to $VMIN_\rho$ and $VMAX_\rho$ at each $x_1$ are plotted with respect to the vertical axis.

Steps 1 and 2 are, respectively, new variations of CVDGs and PVV plots, while Step 3 is a new supplemental plot that can track within the design space where $VMIN_\rho$ and $VMAX_\rho$ occur.

**Example 1.** Let’s return the 16-point BBD and CCD given in Figure 1. Their VDGs in Figure 1 and FDS plots in Figure 3 can be supplemented with their FVDGs shown in Figure 4 (each of which contains 20000 random points). Because of design symmetry
(i.e., permuting \( x_1, x_2, x_3 \) yields the same design), only the FVDG for \( x_1 \) is presented for each design for the second-order model. Design symmetry ensures the FVDGs will have the same \( V(x|x_i = a), VMIN(x|x_i = a) \), and \( VMAX(x|x_i = a) \) curves for \( x_1, x_2, \) and \( x_3 \). What will vary are the locations of the random points. For a large sample of random points, however, the density patterns between the \( VMIN(x|x_i = a) \), and \( VMAX(x|x_i = a) \) curves will be very similar. The plots will also be similar because of the completeness of the second-order model with respect to containing all first-order, interaction, and squared terms. This will not be the case, in general, if a reduced model in which terms were removed. For example, if the squared \( \beta_{11} x_1^2 \) term was removed, the FVDG for \( x_1 \) would be different than the FVDGs for \( x_2 \) and \( x_3 \).

The prediction variance is less stable for the BBD for most values of each \( x_i \). In particular, near \( x_i = 0 \) for \( i = 1, 2, 3 \) there is very large variability in SPV values for the BBD while the SPV remains within a band of approximately ±1.3 for the CCD. The associated maximum SPVs and \( G \)-efficiencies are 16 and 62.5% for the BBD and 10.57 and 94.6% for the CCD. This example highlights a direct comparison of the SPV properties for two competing designs.

**Example 2.** Figure 5 contains the FVDG for the 15-point face-centered CCD with 20000 random design points. Because of design symmetry, only the FVDG for \( x_1 \) is presented for the second-order model. From the FVDG we can study the distribution of \( V(x) \) throughout the cube \( \mathcal{R} \). Figure 5 shows the high density of SPV values near the minimum. Thus, for any \( x_1 \) value, the distribution of SPV values is strongly right-skewed for any \( x_1 \) value. Also, the smallest SPV values will be centered around \( x_i = 0 \), and more specifically, for approximately \(-0.6 < x_i < 0.6 \) for \( i = 1, 2, 3 \).

Across the set of FVDGs, the maximum SPV values will always be equal. The same is true for the minimum SPV values. From the FVDGs for the second-order model in Figure 5, we see that the maximum SPV = 12, and it occurs at each of the 8 vertices \((±1, ±1, ±1)\) (which correspond to the endpoints in each FVDG). The \( G \)-efficiency of a design is defined as \( 100 \times (p/GMAX)\% \) where \( p \) is the number of model parameters and \( GMAX \) is the maximum scaled prediction variance in the design region. Thus, FVDGs provide us with \( GMAX = 12 \), and because \( p = 10 \), the \( G \)-efficiency is 83.3% for this CCD. Although \( G \)-efficiencies can also be determined from and VDGs and FDS.
plots, those plots provide no information regarding where in the design space the largest SPVs occur, which, in turn, provides where prediction variances are poorest in the design space. This an important practical benefit of FVDGs.

CTPs of the coordinates for $V_{MIN_p}$ and $V_{MAX_p}$ are presented in Figure 6. Again, because of design symmetry, it suffices to only consider $x_1$. Due to the design symmetry, $x_2$ and $x_3$ are both interchangeable when calculating the SPV at any given $x_1$. This is seen by the superimposition of the solid and dashed lines in Figure 6a. Thus, if $V_{MIN_p}$ or $V_{MAX_p}$ occurs at a specific $(x_2, x_3)$, it will also occur at the four $(\pm x_2, \pm x_3)$ pairs. Figure 6a shows that $V_{MIN_p}$ occurs when (approximately) $.42 < x_2, x_3 < .57$ or $-.57 < x_2, x_3 < -.42$. The CTP for $V_{MAX_p}$ in Figure 6b indicates that the maximum SPV occurs at $x_2, x_3 = \pm 1$ for any value of $x_1$. Thus, for $x_1$ there are four ridges for both the minimum and maximum SPV that correspond to the signs of $x_2$ and $x_3$. The corresponding CTPs for $x_2$ and $x_3$ are the same as $x_1$ but just with a permutation of the subscripts.

**Example 3.** Consider the 10-point 3-factor symmetric Notz design in Table 1a. Because this Notz design is symmetric, it is sufficient to consider the FVDG for just one of the

![Figure 6. CTPs for the Face-Centered CCD. Solid line ——— for $x_2$ and dashed line - - - - - for $x_3$.](image-url)

**Table 1.**

(a) 10-Point Notz Design

| $x_1$ | $x_2$ | $x_3$ |
|------|------|------|
| ±1   | ±1   | −1   |
| −1   | ±1   | 1    |
| 1    | −1   | 1    |
| 0    | 0    | 0    |
| 0    | 0    | 1    |

(b) 16-point Optex Design

| $x_1$ | $x_2$ | $x_3$ |
|------|------|------|
| ±1   | ±1   | ±1   |
| −1   | 0    | −1   |
| 1    | 1    | 0    |
| 0    | 1    | ±1   |
| .1   | −1   | 0    |
| .1   | −1   | −1   |
| −1   | −1   | 1    |
| 1    | .1   | 0    |

|factor level| coordinate trace for minimum SPV| coordinate trace for maximum SPV|
|---|---|---|
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$x_i$ (e.g., just $x_1$). The maximum SPV occurs at $(x_1, x_2, x_3) = (1, 1, 1)$. Note that this point is the only one of the 8 cube vertices that is not in this design. Therefore, it is expected that the prediction variances at (1) and neighboring points will be large. The FVDG in Figure 7a with 20000 random design points supports that claim.

Suppose that we augment this Notz design by adding the missing vertex design point (1). The design is still symmetric so only one FVDG is needed. The impact of adding this point on the FVDG is clearly seen in the updated FVDG in Figure 7b. Note the stability (i.e., low volatility) in the prediction variances across all values of $x_i$ for $i = 1, 2, 3$ once this vertex is added. This is an example of how FVDGs can be used to assess the impact of design augmentation on the distribution of SPVs in the design space.

**Example 4.** In the third example, consider the 16-point 3-factor nonsymmetric $D$-optimal design generated by SAS Proc Optex (Table 1b) assuming the second-order model:

$$f(x) = \beta_0 + \sum_{i=1}^{3} \beta_i x_i + \sum_{i=1}^{3} \beta_{ii} x_i^2 + \beta_{12} x_1 x_2 + \beta_{13} x_1 x_3 + \beta_{23} x_2 x_3$$

Suppose that we also want to assess the prediction variance properties for “reduced” models, specifically, for the interaction model

$$f(x) = \beta_0 + \sum_{i=1}^{3} \beta_i x_i + \beta_{12} x_1 x_2 + \beta_{13} x_1 x_3 + \beta_{23} x_2 x_3$$

or for the first-order model

$$f(x) = \beta_0 + \sum_{i=1}^{3} \beta_i x_i.$$  

Because the design is not symmetric, the FVDGs for $x_1$, $x_2$ and $x_3$ will differ. Note that the 20000 prediction variances are dense near average $V_\rho$ for the second-order model, while they are dense near the minimum $V_{MIN}(x|x_i=a)$ for all values of $a$ for
For the second-order model in Figure 8a, the small variations in FVDGs occur primarily because the design contains points having $x_1 = \pm 0.1$ as well as $x_2 = \pm 0.1$ while it is not the case for $x_3$. For the interaction model, the FVDGs in Figure 8b highlight the dramatic changes that can occur when a different model is considered. The FVDGs change from quartic to quadratic polynomial shapes. When no squared terms are considered, the smaller SPV values are smaller when compared to the second-order model which is not surprising given that three fewer parameters are estimated. Similar results occur when the model is further reduced to the first-order model with the FVDGs shown in Figure 8c. The associated maximum SPVs, model parameters, and $G$-efficiencies are 13.67, 10, and 73.15% for the second-order model, 12.76, 7, and 54.84% for the interaction model, and 5.77, 4, and 69.37% for the first-order model. This shows that the ordering of $G$-efficiencies is not necessarily related to the number of model parameters. This example highlights the usefulness of FVDGs to assess the robustness of a proposed design due to model reduction or possible model misspecification.

CTPs of the coordinates for $V_{MIN}$ and $V_{MAX}$ are presented in Figure 9. These plots highlight what can happen with a non-symmetric design. Specifically, there may be continuous behavior over an interval, but then a discontinuity occurs. For example, there are discontinuities at $x_1 = .94$ and $x_2 = -.91$ for $V_{MIN}$ and at $x_1 = -.44, x_2 = .46$, and $x_3 = -.75, - .22$ and .69 for $V_{MAX}$. These discontinuities arise because there are multiple local ridges generating SPVs between $V_{MIN}$ and $V_{MAX}$. Then at some $x_i$, one of the local ridges has SPV values that surpass the current minimum or maximum SPV, and a new ridge takes over.

Example 5. Suppose the design space $\mathcal{R}$ is spherical:

$$\mathcal{R} = \left\{ x = (x_1, x_2, ..., x_k) : \left( \sum_{i=1}^{k} x_i^2 \right) \leq \sqrt{k} \right\}$$

Consider the symmetric 15, 16, and 17-point Central Composite Designs (spherical CCDs) having $n_c = 1, 2, 3$ center points, respectively. Therefore, $-\sqrt{3} \leq x_i \leq \sqrt{3}$ for $i = 1, 2, 3$. Again, the design is symmetric, so it is sufficient to consider the FVDG for just one $x_i$, say $x_1$ for the second-order model.

Figure 10 contains the FVDGs with 20000 random points for both the scaled prediction variance $V(x)$ in column 1 and the unscaled-by-$N$ prediction variance $V_1(x)$ in column 2. At either extreme $x_1 = \pm \sqrt{3}$, only one point is in the design space. Thus, the minimum, maximum, and average prediction variances are the same at the endpoints. If you move $x_1$ a distance $\delta$ from these endpoints, i.e., at $x_3 = -\sqrt{3} + \delta$ or $x_3 = \sqrt{3} - \delta$, the minimum, maximum and average SPV or unscaled PV at $x_1 = x_3$ are determined over a large systematic set of points in a circle $\mathcal{C} = \{(x_2, x_3) : x_2^2 + x_3^2 \leq (1 - x_3^2)\}$. That is, the sphere is sliced perpendicularly at $x_3$.

Note the effect of additional center points in the FVDGs for $x_i$ near 0. For $n_c = 1$, the maximum prediction variance occurs at the origin $(0,0,0)$. Then, if $n_c$ is increased to
either 2 or 3, then the prediction variance around (0,0,0) are dramatically reduced. For this example, we recommend comparing the FVDGs for the unscaled-by-$N$ prediction variances because we can assess the direct impact on actual predictions variance unweighted by the design size. In column 2 of Figure 10, there is a clear reduction in $V_1(x)$ around (0,0,0), very little change in the largest $V_1(x)$ values near $x_1 = \pm 1$, and a reduction from approximately.45 to.35 for the minimum $V_1(x)$ values.

The associated maximum SPVs and $G$-efficiencies are 15 and 66.6% for the quadratic model, 10.57 and 94.6% for the interaction model, and 11.231 and 89.0% for the first-order model. Note that the $G$-efficiency increases when going from $n_c = 1$ to $n_c = 2$ because the worst SPV occurred at (0,0,0) when $n_c = 1$ and that is exactly where we

Figure 8. FVDGs for a 16-Point Proc Optex Design for the second-order, interaction, and first-order models.
would collect another data point. There is, however, a diminishing impact when going from \( n_c = 2 \) to \( n_c = 3 \) because \((0,0,0)\) is no longer the point of maximum SPV. Thus, \((0,0,0)\) is not the most \( G \)-efficient point to collect another data point. This does not mean that adding a third center point does not have a positive impact. This can be seen by looking at the unscaled-by-\( N \) FVDGs in which the maximum SPV remains relatively unchanged but the minimum prediction variances are now smaller when comparing the \( n_c = 3 \) to the \( n_c = 2 \) case – another reason to also consider the unscaled-by-\( N \) FVDGs for design augmentation problems.

![Figure 9. CTPs for a Proc Optex Design for the second-order model. Solid line ——— for \( x_1 \), dashed line - - - - for \( x_2 \), and dotted line - - - - - for \( x_3 \).](image-url)
3. Modified componentwise variance dispersion graphs

In the previous examples, it is assumed that the factor levels in an experimental design can be varied independently of each other. In mixture experiments, the factors are the components or ingredients of a mixture, and we assume that the response \( y \) depends
only on the proportions of each component in the mixture. Suppose the mixture has \( q \) components. Let \( x_i \) \((i = 1, 2, \ldots, q)\) be the proportion of component \( i \) in the mixture. The mixture design space will be a subspace of the simplex defined by: \( \sum_{i=1}^{q} x_i = 1 \) and \( 0 \leq x_i \leq 1 \). Note the factor levels cannot be varied independently of each other because \( x_q = 1 - \sum_{i=1}^{q-1} x_i \). Typically there will be a lower limit \( L_i > 0 \) and/or an upper limit \( U_i < 1 \) for component \( i \). In general, the constraints for component \( i \) can be written as \( L_i \leq x_i \leq U_i \) such that \( L_i \geq 0 \) and \( U_i \leq 1 \). For more information of models for mixture experiments, see Cornell (2002) and Smith (2005).

Borkowski (2006) introduced the componentwise variance dispersion graph (CVDG) that summarizes \( V(x) \) throughout a mixture design space. A CVDG for the \( i^{th} \) component is generated from the following four steps. CVDGs are generated for each of the \( q \) components in the mixture.

1. Create an equispaced set of \( x_i \) values \( A = \{ L_i, L_i + \Delta, L_i + 2\Delta, \ldots, U_i - \Delta, U_i \} \). For example, if \( .3 \leq x_i \leq .8 \) with spacing increment \( \Delta = .001 \), then \( x_i \in \{ .3, .301, .302, \ldots, .799, .8 \} \).
2. Fix the component proportion \( x_i = a \) for a given \( a \in A \). Let \( V(x|x_i = a) \), \( VMIN(x|x_i = a) \), and \( VMAX(x|x_i = a) \) be the average, minimum, and maximum of \( V(x) \) conditioned on \( x_i = a \) for all allowable mixtures with \( x_i = a \). Thus, \( \sum_{j\neq i} x_j = 1 - a \).
3. Perform Step 2, for each \( a \in A \). The CVDG for the \( i^{th} \) component is a plot of \( V(x|x_i = a) \), \( VMIN(x|x_i = a) \), and \( VMAX(x|x_i = a) \) across the set of \( x_i = a \) values.
4. Perform Steps 1 to 3, for each of the \( q \) components of the mixture.

In Step 5, CVDGs are modified by incorporating PVV plotting to create a modification of the CVDGs in Borkowski (2006). These new graphs will be called PVV-CVDGs.

1. Calculate \( V(x) \) for a large number of randomly-generated points in the constrained mixture space. Superimpose these points on a CVDG to form a PVV-CVDG.
2. (Optional) Generate CTPs associated with \( VMIN(x|x_i = a) \) and \( VMAX(x|x_i = a) \) for each component proportion \( x_i \). For example, the CTP for \( x_1 \) will have \( x_1 \) on the horizontal axis. The proportions (or coordinates) of the other component proportions \( x_i \) that correspond to \( VMIN(x|x_i = a) \) and \( VMAX(x|x_i = a) \) at each \( x_1 \) are plotted with respect to the vertical axis.

The PVV-CVDGs present a picture of the variability in the entire mixture design space. When producing PVV-CVDGs, it is necessary to use a small increment \( \Delta \) when discretizing the interval \((L_i, U_i)\) for \( 1 \leq i \leq q \) to ensure the maximum of \( V(x) \) in the plots will be close to the true maximum of \( V(x) \) over the entire mixture design space.

**Example 6.** Consider the 3-component poultry feed mixture or “blend” (Smith 2005) with components maize \((x_1)\), fish \((x_2)\), and soybean \((x_3)\) such that \( .3 \leq x_1 \leq .8, 0 \leq x_2 \leq .3, \) and \( 0 \leq x_3 \leq .5 \). Figure 11 shows the triangular coordinate points in the irregularly-shaped polygon within the simplex for two 3-component 14-point mixture designs (Design 1 and Design 2).
Figure 12 contains the PVV-CVDGs for the 3 components for the two mixture designs shown in Figure 11 and assuming the quadratic Scheffé model 

\[ y = \sum_{i=1}^{3} \beta_i x_i + \sum_{i=1}^{3} \sum_{j=i+1}^{3} \beta_{ij} x_i x_j + \epsilon. \]

Note that PVV-CVDGs begin at \( L_1 = 0.3 \) and ends at \( U_1 = 0.8 \) for \( x_1 \), begin at \( L_2 = 0 \) and end at \( U_2 = 0.3 \) for \( x_2 \), and begin at \( L_3 = 0 \) and end at \( U_3 = 0.5 \) for \( x_3 \). The addition of 10000 random points in the PVV-CVDGs provides useful information about the distribution of SPVs within the mixture space that is not provided in the original CVDGs of Borkowski (2006).

For the set of PVV-CVDGs, the maxima across the \( \text{VMAX}(x|x_i = a) \) will always be equal, and the minima across \( \text{VMIN}(x|x_i = a) \) will always be equal (for \( i = 1, 2, \ldots, q \)). From the PVV-CVDGs for the quadratic model, we see that the maxima of \( V(x) \) are 10.8 and 7.8 for Designs 1 and 2, respectively, and occur at the same mixture \( (x_1, x_2, x_3) = (.3, .2, .5) \). Therefore, the \( G \)-efficiencies are 55.6% for Design 1 and is 76.9% for Design 2.

CTPs of the mixture component proportions in Design 2 for \( \text{VMIN}(x|x_i = a) \) and \( \text{VMAX}(x|x_i = a) \) are presented in Figure 13. These plots highlight happens with mixture designs having varying bounds on the component proportions that produce an irregular polyhedron design space within a simplex. There are multiple discontinuities for each \( x_i \) given the multiple local ridges between \( \text{VMIN}(x|x_i = a) \) and \( \text{VMAX}(x|x_i = a) \) produced within the polyhedron.

4. Concluding remarks

To determine which response surface design to run, the experimenter should study the prediction variance properties of each design. We can compare designs using design optimality criteria (e.g., \( D \) or \( G \)). These criteria, however, provide no information about the distribution of the prediction variance function over \( \mathcal{R} \). To address this weakness, graphical methods were developed (e.g., VDGs, PVV, FDS plots, and now FVDGs, CTPs, and PVV-CVDGs), which provide information about the prediction variance properties of a design throughout the design space.

Specifically, FVDGs and CTPs provide useful information on the distribution of prediction variances across the design space. Although \( G \)-efficiencies can be determined
from and VDGs and FDS plots, they do not provide information regarding where in the design space the largest SPVs occur, which, in turn, provides where prediction variances are poorest in the design space. This an one important practical benefit of FVDGs.

FVDGs and CTPs can also be used to (i) assess the robustness of a proposed design due to model reduction or possible model misspecification, and (ii) understand the impact of design augmentation on prediction variance properties within the experimental design region.

Figure 12. Quadratic mixture model CVDGs for the three components of the poultry feed mixture. The first and second columns contain CVDGs for Design 1 and Design 2, respectively. The rows correspond to component proportions $x_1$ (maize), $x_2$ (fish), and $x_3$ (soybean).
Before running an experiment it is recommended to look at multiple graphical tools for studying the prediction variance properties of potential designs to aid in the design selection process. All of the graphical methods help the experimenter to understand \( V(x) \) throughout the design space. Thus, the use of these graphical methods (such as FVDGs and CTPs) is a practical way to compare the prediction variance properties of competing designs.

![CTPs for Design 2 for the quadratic mixture model](image)

**Figure 13.** CTPs for Design 2 for the quadratic mixture model. Solid line — for \( x_1 \), dashed line —— for \( x_2 \), and dotted line ——– for \( x_3 \).
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