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An instance of negative variance-like 'components' in optics by way of applying multivariable calculus to a statistical problem

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Abstract

In the field of optics, the design of a lens often involves analyses of the variability in an optical parameter (such as lens focal length) under manufacturing conditions, which is done in order to identify sources of high variability that may cause the optical parameter to be out of its specification. In this interdisciplinary paper, the author shares his experience in lens design, where analyses of variability are often performed through examining the partial derivatives in a multivariable Taylor series expansion of an optical parameter to second order when interactions are expected. It is shown algebraically that when the second-order expansion is applied to express a sum of squares, negative terms in the sum can occur. This instance of negative-valued "variance-like components" is interesting pedagogically in applied mathematics and statistics, as well as from an engineering standpoint, as it suggests that, based on theory, the variance of a function of random variables may not necessarily be comprised of a simple sum of positive-valued squared deviations comprising its total variance.

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1. Introduction

In engineering, the standard practice of analyzing and assigning permissible variability to factors and parameters is known as "tolerancing analysis", and the permissible values of variability are called, "tolerances" [1]. In the field of optics, particularly, in lens design, an "optical tolerancing analysis" is performed to assign permissible tolerances to

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all variables (factors) that are determined at the factory to have the most significant influence on the optical parameter [e.g., 2-5]. In this paper, the terms "factors" and "variables" are used synonymously, and the term "parameter" is taken to mean some quantity that is a function of multiple variables. The effective focal length (EFL) for a basic telephoto lens, for instance (Figure 1), is a known function of the focal lengths of its two individual lenses, as well as the distance separating the individual lenses [e.g., 6]. If u is the focal length of the first lens, v is the focal length of the second lens, and s is the separation length between the two lenses, then the EFL F of the telephoto lens is given by:

$$\frac{1}{F} = \frac{1}{u} + \frac{1}{v} - \frac{s}{uv}. \tag{1}$$

In the design of a telephoto lens, the magnification of a distant scene is provided by way of selecting values for u, v and s such that F possesses a large value, compared to the focal lengths of common photographic camera lenses (dividing F by a camera lens's focal length yields the magnification). According to Eq. (1), it is clear that even when the EFL of a telephoto lens has been fixed by design (i.e., the values for u, v, and s have been selected), manufacturing processes can cause u, v, and s to vary and hence, result in values of F that are beyond specification. For this reason, a tolerancing analysis is performed to decide on appropriate limits for permissible variability, resulting in the assignment of minimum and maximum specifications (i.e., the tolerances) for u, v, and s. But unlike statistical problems involving the analysis of variance (ANOVA), since Eq. (1) is known, a lens designer need not perform a statistical design of experiments and apply a random effects model to estimate the relative

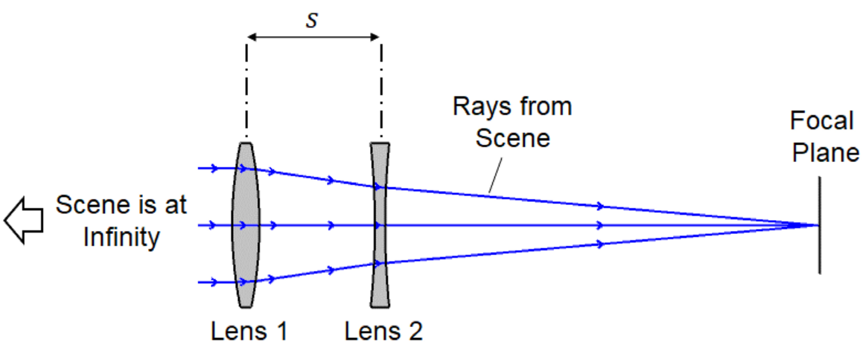

Figure 1

Typical layout (sideview) for a basic telephoto lens, which is comprised of two thin lenses separated by length *s*.

contributions of variance components. Rather, one often performs a combination of error propagation and Monte Carlo simulations [e.g., 2, 3] directly to the formula for a parameter, such as Eq. (1) (in this case, the parameter in the equation is considered a function of random variables). In the case of more complicated systems of lenses where a formula for a parameter may not be expressible in closed-form, one often uses a professional computer-aided design (CAD) program to model optical systems and numerically determine parameter values as a function of input variables. The lens designer lets the program perturb all lens variables in a Monte Carlo fashion, and the CAD program outputs a histogram of resulting parameter values. From such histograms, one examines the spread in parameter values as a consequence of the spreads of individual variables. However, in a lens system Monte Carlo simulation, all variables are perturbed simultaneously at random levels (under an assigned probability density function assumed by the lens designer), so there are no "cross classification tables" that partition the variations. For instance, if there are two variables, such as in Eq. (1) if s is held constant, then there is no table generated where the levels of variable u can be paired with the levels of variable v, as is done in a two-way random effects model ANOVA with crossed classification and interaction in order to partition variability [e.g., 7]. Therefore, in a Monte Carlo simulation in optical tolerancing analysis, there remains the challenge of determining which variables contribute the highest degree of parameter variation such that those variables should be assigned "tighter control" to their variability in the factory. Ordinarily, this problem is handled by using the CAD program to compute first-order partial derivatives of the parameter with respect to its variables and examine the resulting relative magnitudes of the derivatives, the idea being that those variables with the highest derivatives contribute the highest parameter variation. But as statisticians know, this analysis does not consider the "interactions" between variables. Actually, professional lens designers know this, and they have developed methods and algorithms in optical CAD software packages that can compute second-order mixed partial derivatives (i.e., the coefficients of the cross-terms in a multivariable Taylor series to second-order) [e.g., 8-10]. As mathematicians know, this is often called the "quadratic approximation" [e.g., 11], where the cross-terms are analogous to the "interactions" between variables in ANOVA.

To recall, given a two-variable function $Q(x, y)$, a quadratic approximation to $Q(x, y)$ is a Taylor series $T(x, y)$ expressed as

$$T(x,y)=Q(x_o,y_o)+\frac{\partial Q}{\partial x}(x-x_o)+\frac{\partial Q}{\partial y}(y-y_o)+\frac{\partial^2 Q}{\partial x\partial y}(x-x_o)(y-y_o)$$
$$+\frac{1}{2}\frac{\partial^2 Q}{\partial x^2}(x-x_o)^2+\frac{1}{2}\frac{\partial^2 Q}{\partial y^2}(y-y_o)^2, \tag{2}$$

where the partial derivatives are evaluated at x_o and y_o. In the context of an optical tolerancing analysis, the function $T(x, y)$ would be considered an approximation to an optical parameter that is a function of two variables. For example, if we apply Eq. (2) to analyze variability in Eq. (1) (assuming that s is fixed), we could let the parameter F be a function such that $F(u,v) \approx T(u,v)$. As each partial derivative is the instantaneous rate of change of the parameter with respect to the optical variables, each partial derivative is a measure of the sensitivity of the parameter to small changes in the variable. To account for interactions, the quantity $\partial^2 Q / \partial x \partial y$ in Eq. (2) provides this information. Thus, as far as the lens designer is concerned, this is all there is in analyzing how much an optical parameter changes for specific changes in optical variables. This is usually followed by performing Monte Carlo simulations to determine the amounts of spreads of the optical parameter, based on iterative choices for the maximum spreads of the optical variables. The tolerancing analysis terminates as soon as, by virtue of the Monte Carlo simulations, the lens designer has determined that final choices for the maximum spread of all optical variables result in a permissible maximum spread of the optical parameter.

So far, so good. But something interesting happens when we pose the question, "In a Monte Carlo simulation, where x and y become independent normal random variables, what is the variance of $T(x,y)$?" This is the subject of the next section, where, as shall be shown (algebraically), the result is that the variance for $T(x, y)$ may contain negative terms, depending on how we express the function $Q(x, y)$.

2. Algebraic analysis of telephoto lens focal length variability

To begin, it is interesting to note that the analysis of variability in Eq. (1) depends on one's choice of representing Eq. (1). For instance, as is well-known by statisticians, sometimes, one may analyze a parameter by defining a new function for that parameter, which may yield a density function that is more easily dealt with (such as the normal distribution). In optics, one often defines a quantity called the "optical power" of a lens by taking the reciprocal of the lens's focal length [e.g., 12]. In this way, one may re-express Eq. (1) as

$$P = U + V - sUV, \tag{3}$$

where $P = 1/F$, $U = 1/u$, and $V = 1/v$. The quantities P, U and V are now the refractive optical powers of the lenses. In other words, for a telephoto lens such as that shown in Figure 1, P is the total optical power of that lens, while U and V are the optical powers of the two individual lenses, respectively. By these definitions, Eq. (3) would embody everything about linear models for the ANOVA and regression. That is, when s is held constant, Eq. (3) is analogous to the linear model for a two-way fixed effects ANOVA, where the quantity sUV would give rise to interaction. If random levels of variability are given to U and V in Eq. (3), we would have a linear model for a random effects ANOVA if each term on the right side of the equation is expected to yield variance components. However, if the optical power definition for focal length is applied to just the term on the left side of Eq. (1), then some new insights are uncovered, as shall now be discussed.

Suppose that the definitions $U = 1/u$ and $V = 1/v$ are inserted back into Eq. (3). Then, we have

$$P = \frac{1}{u} + \frac{1}{v} - \frac{s}{uv}, \tag{4}$$

where P is the optical power of a telephoto lens. From a lens designer's standpoint, this is intuitively reasonable, as one may be interested to analyze a telephoto lens's optical power as a function of focal length variations in its two constituent lenses. If we now apply Eq. (2) to (4) by making the approximation $P(u,v) \approx T(u,v)$, we have

$$\begin{aligned} T(u,v) = {} & P(u_o, v_o) + A(u-u_o) + B(v-v_o) + C(u-u_o)(v-v_o) \\ & + D(u-u_o)^2 + E(v-v_o)^2, \end{aligned} \tag{5}$$

where the coefficients are

$$A = \frac{\partial P}{\partial u} = -u_o^{-2}\left(1 - \frac{s}{v_o}\right), \tag{6}$$

$$B = \frac{\partial P}{\partial v} = -v_o^{-2}\left(1 - \frac{s}{u_o}\right), \tag{7}$$

$$C = \frac{\partial^2 P}{\partial u \partial v} = -s(u_o v_o)^{-2}, \tag{8}$$

$$D = \frac{1}{2}\frac{\partial^2 P}{\partial u^2} = u_o^{-3}\left(1 - \frac{s}{v_o}\right), \tag{9}$$

$$E = \frac{1}{2}\frac{\partial^2 P}{\partial v^2} = v_o^{-3}\left(1 - \frac{s}{u_o}\right). \tag{10}$$

In the design of telephoto lenses, the focal length of the first lens is always positive (i.e., $u_o > 0$), while the focal length of the second lens is always negative (i.e., $v_o > 0$), and the separation between them is often less than both of the focal lengths (i.e., $|s| < |u_o|$, and $|s| < |v_o|$) [e.g., 13, 14]. A typical telephoto lens design could have, for example, $u_o = 58.52$ mm, $v_o = -95.66$ mm, and $s = 18.84$ mm, which yields $P = 0.01\ \text{mm}^{-1}$, or, equivalently, $F = 1/P = 100$ mm, which is a typical EFL for a telephoto lens that is meant for a 35-mm camera [14]. The point is that, for telephoto lenses, due to the fact that $v_o < 0$, this results in $E < 0$ in Eq. (10). In this case, Eq. (5) becomes

$$\begin{aligned} T(u,v) = {} & P(u_o, v_o) + A(u - u_o) + B(v - v_o) + C(u - u_o)(v - v_o) \\ & + D(u - u_o)^2 - E(v - v_o)^2. \end{aligned} \tag{11}$$

Now, suppose that in a Monte Carlo simulation, we let a program assign k normal independent values (levels) for the variable u, and k normal independent values (levels) for the variable v, where the mean for u is u_o, and the mean for v is v_o (this is done in a typical optical tolerancing analysis, where, as mentioned, unlike standard random effects ANOVA with two factors, there is no attempt to have a cross classification table pairing levels between the variables). Then, we would have k resulting values for $T(u_i, v_i)$, where $i = 1, 2 \ldots k$. The mean of $T(u_i, v_i)$ may then be expressed as

$$\begin{aligned} \overline{T(u_i, v_i)} = \tfrac{1}{k}\textstyle\sum_{i=1}^{k} T(u_i, v_i) \equiv \overline{T} = {} & P(u_o, v_o) + \overline{D(u_i - u_o)^2} - \overline{E(v_i - v_o)^2} \\ = {} & P(u_o, v_o) + \delta d - \delta e, \end{aligned} \tag{12}$$

where $\delta d = \overline{D(u_i - u_o)^2}$ and $\delta e = \overline{E(v_i - v_o)^2}$ are the means for the respective terms. In arriving at Eq. (12) from (11), we note that all odd-powered terms vanish when we compute the mean of $T(u_i, v_i)$, by virtue of having independent normal numbers for u_i and v_i. In an attempt to quantify variability of telephoto lens powers in the Monte Carlo simulation, suppose we now define a deviation of $T(u_i, v_i)$ about its mean as the difference given by $T(u_i, v_i) - \overline{T}$. Then, we would have

$$\begin{aligned} T(u_i, v_i) - \overline{T} = {} & A(u_i - u_o) + B(v_i - v_o) + C(u_i - u_o)(v_i - v_o) \\ & + D(u_i - u_o)^2 - E(v_i - v_o)^2 - \delta d + \delta e. \end{aligned} \tag{13}$$

Now, squaring both sides of Eq. (13), followed by summing the squares, we have

$$\begin{aligned} \textstyle\sum_{i=1}^{k}[T(u_i, v_i) - \overline{T}]^2 = {} & \textstyle\sum_{i=1}^{k}[A^2(u_i - u_o)^2 + B^2(v_i - v_o)^2 + C^2(u_i - u_o)^2(v_i - v_o)^2] \\ & + \textstyle\sum_{i=1}^{k}[D^2(u_i - u_o)^4 + E^2(v_i - v_o)^4 + (\delta d)^2 + (\delta e)^2] \\ & + \textstyle\sum_{i=1}^{k}[-2DE(u_i - u_o)^2(v_i - v_o)^2 - 2D(u_i - u_o)^2(\delta d) \\ & \quad + 2D(u_i - u_o)^2(\delta e)] \\ & + \textstyle\sum_{i=1}^{k}[2E(v_i - v_o)^2(\delta d) - 2E(v_i - v_o)^2(\delta e)]. \end{aligned} \tag{14}$$

What is observed is the presence of negative terms (and hence, negative sums of squares) in Eq. (14). Since the negative terms are in a sum of the squares of differences, they are somewhat like the "components" of a total sum of squares. Hence, perhaps they are proportional to "negative variance-like" components in a total variance (the proportionality constant being a number given by an appropriate way to compute the degrees of freedom).

3. Interpretation of the negative terms

In any Taylor series, there can sometimes be positive and negative terms. If we let the series add up all terms, then provided that the series converges, the Taylor approximation leads to the actual function that it is approximating. By this reasoning, the negative terms in Eq. (14) are just consequences of having a second-order Taylor series expansion. Due to the even-numbered power of the quadratic terms (comprising normal random variables), when the difference $T(u_i, v_i) - \overline{T}$ is squared and summed, there remains at least one negative term that is a function of the variables u and v. Since these two variables are given random independent levels under a normal distribution, the sum of the square of $T(u_i, v_i) - \overline{T}$ does not eliminate the cross-product between the quadratic terms. This implies that the variability given by the sum of the squares of $T(u_i, v_i) - \overline{T}$ is not as high as would be expected when performing a "tolerance stack" computation. In engineering, it is common to perform a sum of squared deviations given by $\sigma^2 = \sigma_1^{\,2} + \sigma_2^{\,2} + \ldots + \sigma_j^{\,2}$, where each of the standard deviations are "errors" or tolerances of, say, the dimensions of parts comprising some device or instrument being integrated to construct, say, a machine, or an instrument. If the deviations are errors in measurement, then the sum is an error propagation [e.g., 15]. If the deviations are tolerances, then the sum is a "tolerance stack" for the dimensions of the parts [e.g., 1], and taking the square root of the total sum yields a so-called "root sum square" (RSS) value to the total dimensional tolerance, which is of course, a total standard deviation. But if a parameter is a function that may be describable by a Taylor series to second order, then there may be negative squared values for at least one deviation, such as implied by Eq. (14), and the total squared deviations [i.e., taking the sum of the squares of $T(u_i, v_i) - \overline{T}$] could be different from that estimated by an RSS calculation. In particular, the sum could be lower than expected from just summing up variance components. In the specific example of deviations of a telephoto lens's refractive power, this seems to be the case. Perhaps this is a physical interpretation of the negative terms in Eq. (14). It is also noted that although it is well-known among statisticians that negative estimates of variance components can occur in statistical analyses of experiments in the ANOVA method based on a linear model, the negative terms in Eq. (14) may not necessarily be related to such occurrences. In particular, one notes that the terms in Eq. (14) are not estimators of statistics, and the quadratic approximation to a parameter is not a linear model for that parameter.

4. Conclusion

The purpose of this paper is to highlight the natural occurrence of negative terms in a sum of the squares of variations given by $T(u_i, v_i) - \overline{T}$ when $T(u, v)$ approximates the formula for a parameter. A specific example has been provided whereby the refractive power of a telephoto lens is regarded as a parameter that is a function of two random variables in a Monte Carlo simulation. When the quadratic approximation is made to this parameter, the result is a number of negative terms in a sum of squared deviations, as shown in Eq. (14). The occurrence of the negative terms in Eq. (14) may serve as a pedagogical example in applied mathematics, statistics, and engineering, where an RSS or a tolerance stack analysis of deviations for a parameter may not necessarily be as large as would be expected.

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