Comment

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This is a thought-provoking article which raises more issues than it answers. The central idea of the paper is to use linear approximations from Taylor's series expansions of size and shape variables in the complex plane. Let the independent Z_i's denote the random locations of landmarks in the complex plane, for $i = 1$ to p. Let μ_i denote the mean of Z_i and suppose the variances of the two independent real and imaginary parts of Z_i are equal for $i = 1$ to p. For $\mathbf{Z} = (Z_1, \cdots, Z_p)'$ and $\boldsymbol{\mu} = (\mu_1, \cdots, \mu_p)'$, let $G(\mathbf{Z})$ be a bona fide size variable, so for $\alpha > 0$, $G(\alpha\mathbf{Z}) = \alpha G(\mathbf{Z})$, and let $H(\mathbf{Z}) = \mathbf{Z}/G(\mathbf{Z})$ be shape, with $H_j(\mathbf{Z})$ the jth coordinate. Let G^* denote the linear Taylor's series approximation of G and H_j^* that for H_j. Now $E(G^*(\mathbf{Z})) = G(\boldsymbol{\mu})$ and $E(H_j^*(\mathbf{Z})) = \mu_j/G(\boldsymbol{\mu})$. Then $\mathrm{Cov}(G^*, H_j^*)$ is used to approximate

$$\mathrm{Cov}(G, H_j) = E(Z_j) - E(G(\mathbf{Z}))E(H_j(\mathbf{Z})).$$

But while $E(G)$ is approximated by $E(G^*) = G(\mu)$ and $E(H_j)$ by $E(H_j^*) = \mu_j/G(\mu)$, $E(Z_j) = \mu_j$ is approximated by $E(G^*H_j^*)$. Note that if $E(Z_j)$ is not approximated, but $E(G)$ and $E(H_j)$ are, then the covariance is zero, regardless of the size variable! Such approximations encourage zero covariances.

The author shows for the "size" variable $S(\mathbf{Z}) = \sum |Z_i - Z_j|^2$ that linearized size is uncorrelated with the linearized version of a different shape variable. One can show for the proper size variable $S^{1/2}$ that the linearized version of it is uncorrelated with shape $\mathbf{Z}/S^{1/2}$. If one only slightly improves the approximation by replacing the linearized variable $S^* = \sum |\mu_i - \mu_j|^2 + dS$ by $S' = \sum |\mu_i - \mu_j|^2 + 2p(p-1)\sigma^2 + dS$, the linearized variable with the correct expectation, one obtains a zero covariance for $p = 3$ only if the triangle is equilateral. I surmise that the more accurate approximation using the quadratic term of the Taylor's series expansion leads to a generally nonzero covariance as well. Of course, in the case in which $\sigma^2/S(\boldsymbol{\mu})$ is quite small, these covariances are quite close to zero.

The issue of zero correlation of linearized size and linearized shape is certainly an idea that merits further exploration. For simplicity, consider the case of p positive random variables rather than the p random complex vectors. Assume the X_i are random variables for $i = 1$ to p. Let $\mathbf{X} = (X_1, \cdots, X_p)'$ and denote $E(\mathbf{X})$ by $\boldsymbol{\mu} = (\mu_1, \cdots, \mu_p)'$ and covariance of $\mathbf{X}$ by $\sum = (\sigma_{ij})$. Let $G(\mathbf{X})$ be a size variable and $H(\mathbf{X}) = \mathbf{X}/G(\mathbf{X}) = (H_1(\mathbf{X}), \cdots, H_p(\mathbf{X}))'$ shape. Let G^* and H_j^* be linearized versions of G and H_j. Then the covariance of G^* and H_j^* depends only on $\boldsymbol{\mu}$ and $\sum$:

$$\mathrm{Cov}(G^*, H_j^*) = \frac{1}{G(\boldsymbol{\mu})} \sum_i \sigma_{ij} \left.\frac{\partial G}{\partial x_i}\right|_{\boldsymbol{\mu}} - \frac{\mu_j}{G^2(\boldsymbol{\mu})} \sum_{i,k} \sigma_{ik} \left.\frac{\partial G}{\partial x_i}\right|_{\boldsymbol{\mu}} \left.\frac{\partial G}{\partial x_k}\right|_{\boldsymbol{\mu}}.$$

When is this zero? If the X_i's are independent and $G(\mathbf{X}) = \sum X_i$, then it is zero provided $\sigma_{ii} = k\mu_i$. However, this does not imply independence of size and shape, for it is well known for independent X_i's that sum size is independent of shape only if the X_i's are gamma random variables with common scale parameter (Mosimann, 1962), in which case $\sigma_{ii} = k\mu_i$. If the X_i's are independent and $G(\mathbf{X}) = (\sum X_i^2)^{1/2}$, then G^* and H^* have zero covariance if σ_{ii} is constant for $i = 1$ to p. But for independent X_i's this size variable is independent of shape only if the X_i^2 are gammas with the same scale parameter; i.e., the X_i's are generalized gammas with the same scale parameter. It is clear that linearized size uncorrelated with linearized shape is much less stringent than size independent of shape. In general, for size to be independent of shape for independent variables, James (1979) has shown that the distribution is generalized gamma or its limiting cases (such as lognormal) and for each distribution there is a particular size variable. What are the two- and three-dimensional analogs of this result?

An interesting unanswered question concerns uniqueness of the size variable such that linearized size is uncorrelated with linearized shape (of course, linearized size is not guaranteed to be a positive random variable). It is clear that the theorem of Mosimann (1970) concerning the uniqueness of the size variable independent of shape as cited by the author does not apply. (That this theorem means that "In other words, although 'size' and 'shape' are verbally orthogonal, computationally and conceptually they are inextricably entangled" is at best debatable.) What is clear is that in general uncorrelated linearized size and linearized shape do not imply linearized size independent of linearized shape and certainly cannot be construed to mean that therefore size is independent of shape, a trap into which the author apparently falls. It is also unfortunate that what is exact and what is approximate in the article is not clearly delineated. Perhaps this is due to the fact that the notion of a

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(stochastic) differential is not carefully defined. For example, it appears that Lemma 1 and the result of the next paragraph are exact expressions when in fact they are only approximate. The complete exact expression for $|\mathbf{Z}_1 - \mathbf{Z}_2|^2$ is:

$$\begin{aligned} |\mathbf{Z}_1 - \mathbf{Z}_2|^2 &= (\mathbf{Z}_1 - \mathbf{Z}_2)\overline{(\mathbf{Z}_1 - \mathbf{Z}_2)} \\ &= \mathrm{Re}\{(\mathbf{Z}_1 - \mathbf{Z}_2)(\bar{\mu}_1 - \bar{\mu}_2)\} \\ &\quad + \mathrm{Re}\{(\mathbf{Z}_1 - \mathbf{Z}_2)(d\bar{\mathbf{z}}_1 - d\bar{\mathbf{z}}_2)\} \\ &= (\mu_1 - \mu_2)(\bar{\mu}_1 - \bar{\mu}_2) \\ &\quad + 2\mathrm{Re}\{(\mu_1 - \mu_2)(d\bar{\mathbf{z}}_1 - d\bar{\mathbf{z}}_2)\} \\ &\quad + (d\mathbf{z}_1 - d\mathbf{z}_2)(d\bar{\mathbf{z}}_1 - d\bar{\mathbf{z}}_2). \end{aligned}$$

Part of this confusion is that the mean of $|\mathbf{Z}_1 - \mathbf{Z}_2|^2$ is not $|\mu_1 - \mu_2|^2$. Of course these approximations for $\sigma^2/|\mu_1 - \mu_2|^2$ very small are quite good and do not affect the covariance calculation.

The underlying theme of this article is that the geometry of landmarks can finally be exploited and that one no longer needs to rely on purely algebraic analyses for shape. Consider this claim for the triangle of landmarks. The shape variable is expressed as the ordered pair (U, V) for the third vertex, where $Q = U + iV$, for the registered triangle. Let D_1, D_2 and D_3 be the random lengths from vertices 1 to 2, 2 to 3 and 3 to 1, respectively. Then

$$U^2 + V^2 = D_3^2/D_1^2;$$
$$(1 - U)^2 + V^2 = D_2^2/D_1^2;$$

so $U = \frac{1}{2}\{1 + D_3^2/D_1^2 - D_2^2/D_1^2\}$ and $V = \pm\{U^2 - (D_3^2/D_1^2)\}$. Thus the map from (U, V) to $(D_2^2/D_1^2, D_3^2/D_1^2)$ is 2 to 1. But if $|Z_i - \mu_i| \ll |\mu_i - \mu_j|$ for $i \neq j$, then the sign of V is unchanging and the map is 1 to 1. In short, by the nature of the assumptions, the geometry is effectively removed from the problem, to be replaced by functions only of distances. It is true that there is geometry in terms like $(Z_i - Z_j)\overline{(Z_k - Z_m)}$ but this information is not exploited nor is it necessary under the assumptions. This reduction suggests that one could just as easily work with the distances. For example, one could suppose that $(D_1, D_2, D_3)/(\sum D_i)$ has a Dirichlet distribution, a model which could accommodate random distances that vary more than a little. Or for the normal model of this paper, the distances of the random lengths, suitably normalized, are noncentral chi distributions and one could inquire as to the distribution of the shape vector $(D_1^2, D_2^2, D_3^2)/S$. Note that the circular error model is absolutely crucial to this latter approach.

Consider the two biological examples offered in the article. The first pertains to a microscopic sea fossil. A glance at Figure 7b immediately indicates that the assumptions of the model of the first part of the paper cannot be met, as the (U, V) do not appear to be circular normal nor is it the case that the standard deviations are small relative to the distances. Therefore, while there appears to be an interesting relationship between size and shape, it does not appear to be pertinent to the prior development of the paper.

Consider the second example concerning the dental x-rays of children at ages 8 and 14. For the two sexes at age 8, it would seem that the validity of the assumptions of the model and the investigation of uncorrelatedness of size and shape would precede analyses of size differences by sex and shape differences by sex. In any case, the model certainly seems reasonable for the males based on Figure 6, even the crucial circular rather than elliptical errors, and the ratio of σ to $|\mu_i - \mu_j|$ estimated from Table 1 appears sufficiently small. It is no surprise then that size and shape do not appear to be correlated and hence the separate investigations for size and shape are appropriate.

The notion of monitoring the same individual at different time points is quite a separate issue. Suppose that the time interval is small so that the standard deviation is small relative to the distances for say two points in space. A little thought will suggest that over time (even small time) that the errors should not be random in every direction but that there is a drift direction whose random length is proportional to the small time change as well as a nondirected random component. The author claims that changes in size and changes in shape can be modelled with his development, in which case under the assumptions of the model, changes in size should be approximately uncorrelated with changes in shape. However, the test for the relationship of size to shape for children ages 8 and 14 indicates that changes in size are correlated which changes in shape, negating the model. Perhaps the time interval of 6 years is too large. Unfortunately, the additional biorthogonal grid approach appears to depend on the validity of the model to span successfully the stochastic spaces for size and shape. The standard deviation relative to the change in distance is quite a bit larger than those at a fixed age, from Table 1. This suggests that a more sophisticated model may be required to model stochastic behavior in repeated measures of landmarks in this portion of the second example.

In any event this paper is sure to stimulate further interest and research in this important area of size and shape in multidimensions.

ADDITIONAL REFERENCES

JAMES, I. R. (1979). Characterization of a family of distributions by independence of size and shape variables. *Ann. Statist.* **7** 869–881.

MOSIMANN, J. E. (1962). On the compound multinomial distribution, the multivariate β-distribution, and correlations among proportions. *Biometrika* **49** 65–82.