Committee II
Theoretical Empiricism: A General
Rationale for Scientific Model-Building

First Draft --
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SPATIAL REPRESENTATIONS IN HYPOTHESIS GENERATION

by

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Discussion Paper

on

Fred Bookstein's

SOFT MODELING AND THE MEASUREMENT OF BIOLOGICAL SHAPE

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1. Introduction

The ideas presented by Bookstein are highly original and thought-provoking. His aim is a reformulation of morphometrics, the development of a geometrical science of shape and its changes. Since he published his 1978 Springer book (Bookstein, 1978), which covers much of the material of this paper in more detail, he has pursued this aim almost single-handedly. This trail-blazing work is beginning to be cited only now and coming to the attention of scientific communities. Alternative approaches that may also be original and promising are now emerging as well (Kolata, 1984).

My discussion of Bookstein's paper addresses four aspects: (1) the form of the paper; (2) its contributions; (3) an assessment of the developing new theory of morphometrics that it illustrates and introduces to this audience; and (4) the intellectual ferment and new ideas it stimulated in me regarding cognitive processing and mental imagery.

2. Form of the paper

The style is erudite and literary. The language is anything but direct and simple. It assumes the reader to have not only a large vocabulary that includes rarely used words such as "adumbrate," "aliquot," "obverse," "transect," but also to know the literature on latent variables, soft modeling, tensor analysis, differential geometry, and transformational analysis. Some assertions are very cryptically presented. To show the reader why, for examples, the formulas of equation (1) for the two shape coordinates of a triangle hold, the author might have provided the reader with a one-line reminder that in Fig. 1, ν_1 is just the projection of AC on AB, which is the inner product of these two vectors divided by the length of

AB, and that the result is to be divided by the length of AB since that is taken to be 1 in the transformed triangle.

The effort to understand this paper and the theory underlying it is rewarded, however, by the new ideas it is likely to stimulate in the reader, the appreciation and insight he is likely to gain into this highly original and useful synthesis of statistics, geometry and computation, and the light it sheds on some of the key issues in the area of soft modeling and theoretical empiricism.

3. Soft Modeling

Bookstein's contribution in this paper is to conceptualize soft modeling as a dynamic process in which the manifestation of latent variables converges as a result of the interplay between improved measurements, covariance modeling and the interpretation of patterns discovered in covariance modeling. This assumes, of course, that more measurements can be taken as needed, which is the case for the experiments he deals with, but not for historical time series.

The argument can be cast in information theoretic terms. With measurements of a point in the plane represented by 2 n-bit numbers, it takes 6n bits to specify a triangle; or to put it differently, if each of 2^{6n} triangles were equally likely, it would take 6n bits to reduce uncertainty to zero about which one was intended. If the perimeter were specified by k bits, then shape would be encoded by 6n-k bits. If the vertices of a triangle denote one of 2^{m} equip~~otential~~robable landmarks, it takes about m additional bits per vertex to indicate which landmark. The residual uncertainty is not zero, however, because of statistical variability. Hence, not all the $6n-k+m$ bits of initial uncertainty are removed by a data set. To remove the remaining uncertainty requires not only more data, but a newly structured data set designed, on the basis of the geometric models for probing into the nature of the uncertainty, to maximally reduce it.

In the examples given, success in applying the proposed morphometric method depends crucially on the existence of consensually accepted landmarks that are readily recognized and assigned to points on a surface. It is not evident that such landmarks exist for all biological shapes. If they exist but are not yet known, then perhaps this method can help in finding them. This is another illustration of the dynamic aspect of soft modeling that Bookstein stresses in this paper.

In general, soft modeling should be regarded as a convergent, dynamic process in which the statistician learns from the data to improve his design and his models, which lead to better data and in turn to better models and designs. The biorthogonal grid suggests new indicators that sketch the latent variables better than other indicators.

4. Biological Morphometrics

The main claim for the new theory, first made in his 1978 book and repeated here, is that the latent variables of biological shape are best represented by a biorthogonal grid, and that changes in shape are best represented by the stretchings or compressions at each point of the grid in the principal (perpendicular) directions. It is this grid and the dilatations in its principal, orthogonal directions which best represents latent shape variables and leads to new indicators that represent the latent variables even better.

Further progress in developing this theory consisted of building connections with statistics, computation and applications. Geometric representations of mean changes in shape as well as statistical deviations from the mean are illustrated in Fig. 8 of Bookstein's paper. An algorithm for determining the biorthogonal grid has been programmed for any shape. These techniques have been applied to the analysis of developmental changes of craniofacial shapes studied by orthodontists, to computed tomographic images to aid radiological diagnosis and in developmental biology. There would also seem to be applications in crystallography, surface science, the analysis of protein-denoting dot patterns from 2-dimensional gel electrophoresis, meteorology, bibliometrics and acquaintance networks, to mention but a few.

A potential use of the theory and the method it supports is to supplement the human eye and human clinical judgments by quantifying the geometry of shape and its changes. The concepts and methods of morphometrics reflect a reductionistic, non-holistic approach through analysis into biorthogonal grids and growth tensors. This restricts the analysis to diffeomorphisms but it will not apply to changes in form illustrated by a blastula that folds and joins onto itself to form topologically different shapes. It does not deal with the kind of singularities studied by R. Thom (Thom, 1975). And it does not completely capture the holism D'Arcy Thompson (1961) may have intended in his search for a "comprehensive law of growth (that) has pervaded the whole structure in its <u>integrity</u>." Topology appears better suited for this program than quantified geometric shape parameters. Of course, there is a tendency to quantify topology as well, as in algebraic topology, and perhaps it is Poincaré's message to think qualitatively about dynamical systems that may best capture Thompson's intent. As long as we use Bookstein's morphometrics in *conjunction* with human judgments or with holistic human perceptions, so that a holistic view always complements the reductionistic approach, a balanced perspective prevails that is likely to avoid error. Perhaps a more global counterpart to Bookstein's morphometrics--"morphodynamics"--will emerge from current research on dynamic systems. (Hirsch, 1984)

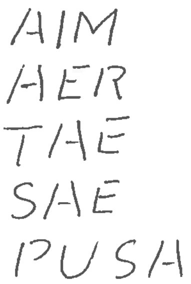
5. Cognitive Processing and Mental Imagery

The claim of morphometrics that dilatations along principal axes of some biorthogonal coordinate grid is the "best" way to represent change in latent shape variable raises the question whether people might use such a representation in categorizing and discrimination tasks, and in hypothesis formation.

Discriminant-Formation. Suppose that a person S is given two piles of objects (that we denote by A and B) and then shown a new object and asked to assign it to A or B according to where he thinks it "fits better." How could he generate hypotheses about what the objects in each pile have in common and about the discriminants that carry the difference. To be specific, suppose A consists of cards with hand-printed words on them:

AND
AUTO
BAND
BOAT
SPA

and B with words such as



If S can read printed English, he might hypothesize that every word in A contains an A and every word in B contains an H. Presence of A could thus be a discriminant. If he assigns the next n cards correctly according to this discriminant, our inferences that he holds this hypothesis may have high validity.

But how can we infer anything about how S generates that hypothesis? It is not the shape of /-\ alone that carries the difference, since it is identical in /-\ND and T/-\E. In this case, it is clearly the context and knowledge that HND and TAE are not ordinarily English words. In scanning the words in A for commonalities, an S who knew the Roman alphabet but no English would not do as well. There are many discriminants other than the "presence of A" inferred by S from context or world knowledge that S might think of using; some might be better than others in explaining commonalities and differences; some might be more elegant than others. The morphometric thesis is not likely to hold here.

Computers have been used to generate hypotheses (Kochen, 1960), and then used to produce responses based on them, for comparison with corresponding responses from human subjects. A perfect fit would justify the inference that the hypothesis-generating algorithm implemented in the computer was the one used by the human subjects provided that there are no other algorithms that produce the same response sequence. Most of the models we used (Kochen, 1982; Kochen and Stark, 1978; Kochen, 1976) involved a dynamic, an algorithm that generates or revises other algorithms. There is more variability in humans, and thus a perfect fit is unlikely.

Spatial representations. A spatial representation is more holistic, less reductionist than one using combinations of attributes and their values. Thus, the image of a snowball carries more information than the statement that is is white, cold, round, will melt if held in warm hands, etc. Even representations like Scripts (Schank and Abelson, 1977), Frames (Minsky, 1975), or E-MOPS (Kolodner, 1983) will not capture completely what a person knows from imaging a snowball. Such images help a person answer and ask many questions and to form hypotheses about how snowballs, snowmen, icicles and popsicles on the one hand differ from baseballs, sculptures, ice cream and stalactites on the other. The prerequisite for making such spatial representations in hypothesis generation may be the ability to shift flexibly between a holistic and an analytic representation, and between global, bird's-eye and local, worm's-eye perspectives in either representation.

Shape variables in synthesizing hypotheses. A major problem in hypothesis-formation is the generation of new predicates and variables. For example, in noticing that 3,4,5 could be sides of a triangle, the concept of perpendicularity might be encountered for the first time. As Bookstein notes, an angle is the simplest example of a shape variable.

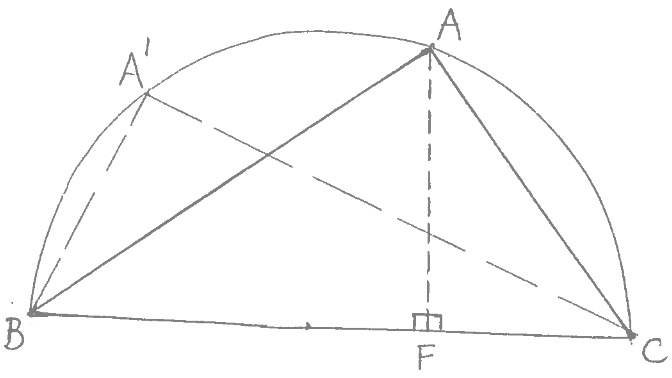


Fig. 1

If we inscribe triangle ABC in a circle, all the angles A, A' are the same, for the same base. If the base goes through the circle's center, then they are all right triangles, as would be the case for a triangle with sides of lengths 3,4 and 5. This can trigger the generation of many construction operators (e.g. an altitude on BC) from which the relation of similarity among three triangles (e.g. BFA, BAC and AFC) may be generated. Changing the shape variable (angle A) only slightly removes the clue that there are similar triangles. If, by chance, a discoverer noted that triangles AFB and AFC combine to make up triangle BAC, and that the areas of these three triangles are proportional to the squares of their longer (corresponding) sides, he might be motivated to generate Figure 2 and with it the theorem of Pythagoras.

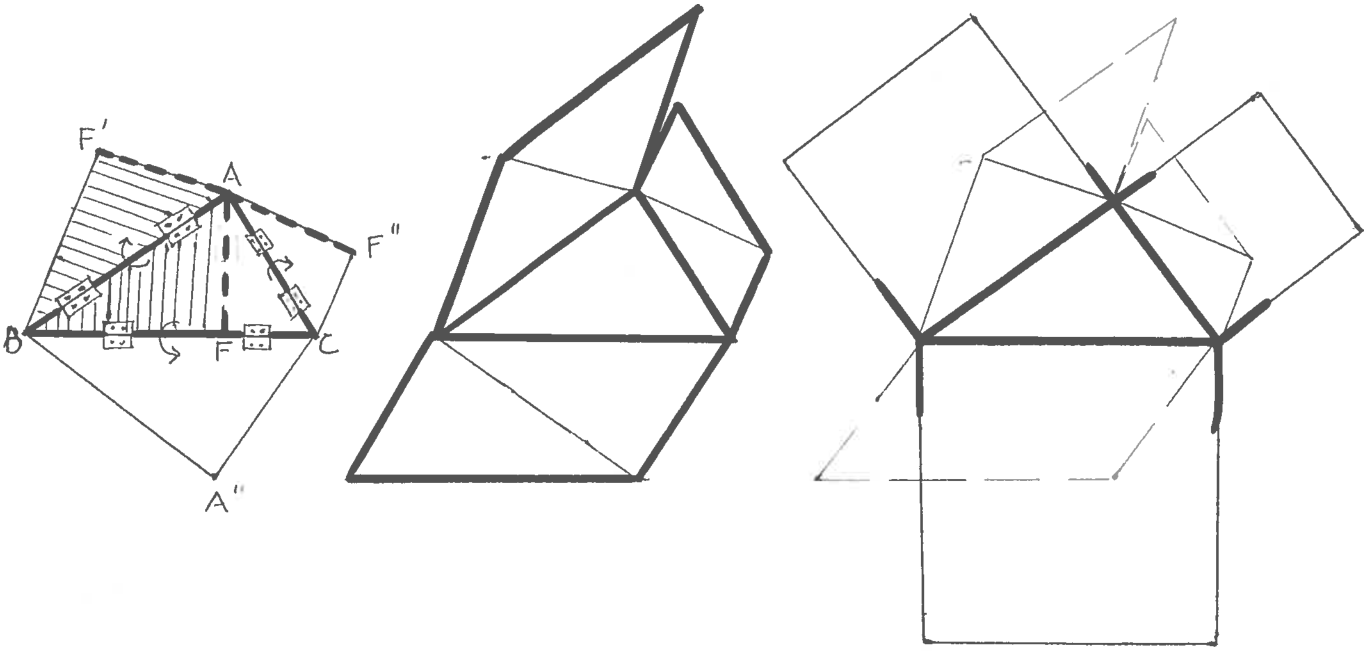


Fig. 2

6. Summary and Conclusion

Bookstein has been developing a new approach to morphometrics--a geometrical science of shape and how it changes--since 1978. His thesis is that dilations at each point along the principal axes of a biorthogonal curvilinear coordinate grid is the best way to represent change in latent shape variables. This claim is substantiated in applications to measuring changes over a decade in an orthodontal patient's craniofacial patterns such as a triangle with vertices at such landmarks such as the bridge of the nose. The dilations can be represented by a strain tensor. Average changes and deviations from the mean can be represented geometrically. The theory supports an algorithm, available as a computer program, for finding an appropriate biorthogonal grid for any given shape. This can be used to supplement the ability of the human eye and of clinicians in making holistic judgments by quantifying the geometry of changing shapes.

In this paper, Bookstein conceptualizes soft modeling as a dynamic process. It is a convergent sequence of manifestations of latent variables. These result from interplay between improved measurements, covariance modeling, and interpretation of patterns discovered in covariance modeling.

This discussion presented some new ideas about hypothesis-formation and spatial imagery that were stimulated by Bookstein's paper. The limitation of the morphometric thesis, with its reductionist bias, are discussed. The contribution of this paper to soft modeling is critically analyzed. The paper is judged to succeed in presenting a synthesis of geometry, statistics, and computations, with a variety of useful applications and potential for opening a new line of inquiry likely to stimulate research.

Bookstein, F.L. The Measurement of Biological Shape and Shape Change (Lecture Notes in Biomathematics), Berlin: Springer, 1978.

Kolata, G. "Esoteric Math Has Practical Result," Science 225, 4661, 3 August 1984, pp. 494-495.

Kochen, M. "An Evolutionary Approach to Concept and Hypothesis Formation," in R. Groner et al (eds.), Methods of Heuristics, Hillsdale: Erlbaum, 1982.

Kochen, M. and Stark, J. "Representation and Formation of Hypotheses in Learning Programs," in Proc. Int'l. Conf. on Cybernetics and Society, IEEE, Tokyo, 1978.

Kochen, M. "On Learning Global Aspects of Shapes," in Proc. Milwaukee Symposium on Automatic Computation and Control, 1976.

Kochen, M. "Experimental Study of Hypothesis-Formation by Computer," in C. Cherry (ed.), Information Theory, London: Butterworth, 1960.

Schank, R.C. and Abelson, R.P. Scripts, Plans, Goals and Understanding, Hillsdale: Erlbaum, 1977.

Minsky, M. "A Framework for Representing Knowledge," in P.H. Winston (ed.), The Psychology of Computer Vision, New York: McGraw-Hill, 1975.

Kolodner, J. "Reconstructive Memory: A Computer Model," Cognitive Science 7, 4, 1983, pp. 243-328.

Thom, R. Structural Stability and Morphogenesis, Reading, MA: Benjamin, 1975.

Thompson, D'A.W. On Growth and Form (orig. 1917, 1942), Cambridge: The University Press, 1961.

Hirsch, M. "The Dynamical Systems Approach to Differential Equations," Bull. Am. Math. Soc. 11, 1, July 1984, pp. 1-64.