

Estimation of ultrastructural relations: a synthesis of the functional and structural models and factor analysis

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Existing expositions of maximum likelihood estimation of the linear functional and structural relations fail to provide insight into the underlying unity of the two models. Moreover, as Gower and Mardia [4] have recently commented: "... the link between structural and factor models seems to be a new and intriguing one". This thesis seeks to give a unified presentation of estimation theory which will embrace all three models. This is accomplished through the following syntheses: first, by showing that for the linear functional relation, maximum likelihood estimation is equivalent to generalized least squares estimation, thus proving a conjecture due to Sprent [8]; second, by considering a new model, the ultrastructural relation, which contains the functional and structural relations as special cases; third, by establishing the algebraic equivalence of two algorithms for iteratively solving the maximum likelihood equations - namely, Fisher's method of scoring and Taylor series linearization - thereby clarifying the connection between methods of estimating explicitly and implicitly defined functional relations.

The thesis begins by considering maximum likelihood estimation of linear or nonlinear functional relations, assuming that replicated observations have been made on p variables at n points. The joint distribution of the pn errors is assumed to be multivariate normal. Known results are extended in two ways: from known to unknown error covariance matrix, and from the bivariate to the multivariate situation.

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In the linear case, the equivalence of maximum likelihood and generalized least squares methods is established.

Next, the connection between the methods of Britt and Luecke [2] and Dolby [3] is investigated. Britt and Luecke postulated a functional relation written in implicit form and used a Taylor series linearization of the fitted function to maximize the likelihood subject to the constraints imposed by the relation. Dolby wrote the functional relation in explicit form, and employed the method of scoring to solve the unconstrained maximum likelihood equations. It is shown that, provided the implicit relation may be recast in explicit form, the two methods are algebraically identical.

Attention is then turned to the bivariate case of the ultrastructural relation. In the replicated context, the slope estimate turns out to be a root of any one of three quadratic equations. The coefficients arising in one of these equations are functions of the between group sample covariances and of $\hat{\lambda}$, the estimate of the ratio of the error variances of the independent and dependent variables, respectively. In the other two forms of the quadratics, the between group covariances are replaced by other sets of covariances, the equations being equivalent because of certain symmetries in the expression for $\hat{\lambda}$. Incidentally, this solves a problem noted in a review paper by Moran [7], namely, the maximum likelihood estimation of the replicated structural relation. In the unreplicated case, it is shown that *two* variance ratios must be known *a priori*, whereupon the slope estimate is a root of a quintic equation. However, when one of these ratios is zero, we obtain an estimator of the slope which is the geometric mean of one predictive regression and the reciprocal of the other. This estimate was proposed on heuristic grounds by Teissier [9] and interested Kermack and Haldane [5] on account of its scale invariance.

The thesis concludes with a generalization of the ultra-structural model to the case of m simultaneous linear relations in p variables and a complementary factor analytic model involving f ($= p-m$) factors. Maximum likelihood estimates of the coefficients of the relations turn out to be solutions of a generalized eigenvector problem involving the within and between groups covariance matrices. A corollary, for the case $m = 1$, is that maximum likelihood estimates of the coefficients of single functional and ultrastructural relations are identical. This provides an explicit solution for one of the functional relation models considered

earlier. The general model, when specialized to its functional and structural cases yields the classical forms of factor analysis due to Whittle [11] and Lawley [6], respectively. It is also shown that the "estimate" of mental factors due to Thomson [10] arises from the model of structural type and is the conditional expectation of the factors given the observations; whereas that of Bartlett [1] is the maximum likelihood estimate of the factors in the model of functional type.

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