Chemometrics, Econometrics, Psychometrics – How Best to Handle Hedonics?

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Abstract

How should consumers' choices and preferences for foods be modeled? How do the taste, color, aroma and texture of a food affect its liking? Sensory scientists may choose models from multiple disciplines for analyzing the relationship of consumer hedonics to the physical, chemical and perceptual characteristics of sensory objects. Two characteristics of sensory hedonics, satiety and differential variation, severely constrain the ability of models that cannot process these characteristics to successfully model this relationship. Overestimation of models with an excessive number of parameters is also shown to be a serious problem.

Keywords: unfolding, PREFMAP, PLS, PROSCAL

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"Hedonics" evokes different associations in different disciplines. In economics, hedonic analysis commonly refers to how product characteristics are priced in the market place. In psychology, hedonics is more likely to have an association with experimental analyses designed to understand how subjects form preferences or make choices. While psychology is not limited to the visual sense, visual attributes are the focus of most sensory studies in psychology. Chemometric studies, like those in psychology, are usually experimental as well. Attributes, though, generally capture the physicochemical properties of products or consumers' sensory perceptions of these properties.

The purpose of this paper is to review some of the distinctive contributions of each discipline, critically look at assumptions on which they are based, and form some hypotheses as to what properties would be most desirable for future hedonic models to possess. Of the three disciplines, the one that has been around the longest and borrowed the least from the others is econometrics. We shall thus start with econometrics, proceed to psychometrics and then chemometrics.

Econometrics

Hedonic prices are defined in economics as the implicit (shadow) prices of product attributes that are revealed from the observed prices of products in the market place. The comparative statics approach to hedonic pricing provides a mathematically elegant means of imputing value to product characteristics. First formulated by Rosen (1974), goods of design z are defined by their n attributes $z_1, \ldots, z_n$. The consumption decision is made by maximizing $U(z,y)$ subject to $P(z) + y = K$ where $U(\bullet)$ is a strictly concave utility function for a good with characteristics $z_1, \ldots, z_n$ and all other goods y which are measured in dollars, $P(z)$ defines the market price of each alternative bundle of characteristics, and K is the consumer's income. The consumer's willingness to pay for z is denoted by $\theta(z)$. Production decisions are made by firms that maximize profit $\pi = M(z)P(z) - C(M, z)$ where $M(z)$ is the number of units produced of design z and $C(M, z)$ is the total cost function. To account for differences in tastes among consumers, the utility function may be generalized to $U(z,y;\alpha)$ where α is a vector of shift variables that characterize the individual consumer. Common shift variables in sensory studies include psychological, socioeconomic, demographic and attitudinal variables. Likewise, the cost function may be expanded to $C(M, z; \beta)$ where β is a vector of technology parameters that vary across firms. $\theta(z)$ and $P(z)$ may also be generalized.

Rosen's model is thus like traditional comparative statics models in economics except that it is framed in terms of characteristics instead of goods. Consumers are assumed to maximize their utility and firms are assumed to maximize their profit. After specifying the functional forms, the utility and profit functions are differentiated with respect to z. Equilibrium prices for characteristics $z_1, \ldots, z_n$ are determined by equating supply and demand. Optimum attribute values z^* are determined where $\theta(z^*) = P(z^*)$. Unknowns are estimated by simultaneously solving a demand and a supply equation for each attribute. These reduced form equations are determined by differentiating $P(z)$ and $\theta(z)$ for each of their n arguments.

While the theoretical richness and mathematical elegance of Rosen's model is undeniable, its appropriateness for designing new sensory products is limited at best. Three reasons for its inappropriateness are the following:

(1) it assumes that only one unit of a product is purchased within a given time period - the model is thus more appropriate for big ticket consumer durables than for packaged goods;

(2) the concave assumption about the utility function means that all characteristics will have non-negative marginal utility – a traditional assumption in economics that unfortunately contradicts the pervasive sensory phenomenon of satiety;

(3) there are severe identification problems in the reduced form equations, the information is insufficient for uniquely estimating the desired equations. Spirited discussions of the identification problem may be found in Brown & Rosen (1982), Eckeland, Heckman and Nesheim (2004) and Epple (1987).

A less comprehensive approach to evaluating hedonic prices is the efficiency frontier method suggested by Lancaster (1966a, 1966b). Instead of following a comparative statics paradigm for hedonic pricing, Lancaster's approach is more analogous to a production process. There is no modeling of the supply side and no assumptions are made about how much a consumer purchases. Instead of finding the good (characteristic bundle) with the highest utility, consumers are said to maximize their utility of characteristics $U(z)$ which could entail purchasing one good or combinations of goods. Goods are transformed into characteristics by means of an objectively measured technology matrix $z = Bx$ where x is a vector of goods. In sensory studies, x would typically be a vector of brands or experimental food products and z would be a vector of product features or attributes. If there were three brands, the quantities consumed would be x_1, x_2 and x_3. The coefficients b_{ij} give the number of units of each attribute z_i supplied per unit of brand j.

As with Rosen, utility maximization is constrained by income, $px \leq K$, where p is a vector of prices. (A more general form of Lancaster's model in which goods are first transformed into activities and then into characteristics is seldom if ever used.) Given a technology matrix and market prices, products can be represented as rays from the origin in a characteristics space – the projection of each ray on a characteristic's axis indicating the magnitude of the characteristics per dollar that a product provides. In Fig. 1, the amounts of z_1 and z_2 per dollar of x_1, x_2 and x_3 are plotted as points A, B, and C which form a concave efficiency frontier in characteristics space. Brand D, which is overpriced, is shut out of the market. A consumer's utility function is assumed to form a convex indifference curve, I. Its point of tangency with the efficiency frontier determines the product or combination of products purchased by the consumer to maximize his or her income constrained utility.

(Please insert Fig. 1 about here.)

Calculation of the efficiency frontier is straightforward if objective data on relevant choice characteristics are available. Indifference curves may be estimated in a variety of ways, usually from experimental data (MacCrimmon & Toda, 1969).

While Lancaster's approach does not have the single purchase limitation of Rosen's method, it shares the non-negative marginal utility assumption. Figure 1 depicts a brand E that exhibits negative marginal utility on characteristic z_1. It could have a higher utility than Brand A but would never be selected by the model because it is off the efficiency frontier. A second limitation is the assumption that satisfaction obtained from characteristics is independent of the goods that deliver them or the combinations in which they are experienced – one cup of tea that is very sweet followed by another that is not sweet produces the same satisfaction as two cups of tea that are mildly sweet (Ackerman, 1997).

While the comparative statics and efficiency frontier approaches are rich in economic theory, it is in the relatively theory free area of hedonic regression analysis that the greatest number of sensory applications are to be found. Hedonic regressions, which use prices as dependent variables and product characteristics as independent variables, grew out of the need to measure quality changes and construct meaningful price indices. Waugh's (1928) study on vegetable prices, which reported how physical characteristics, such as size, shape, color, maturity and uniformity influenced the prices of asparagus, tomatoes and hothouse cucumbers, was the first empirical study to relate price and quality. An historical review of hedonic regression research is provided in Chapter 4 of Berndt (1991).

Like the previously cited econometrics approaches, hedonic regressions avoid the biases of survey response methods associated with psychometric studies by evaluating market place data. Hedonic regressions have the potential to explicitly model effects such as negative marginal utility and interactions among characteristics. However, most "are typified by their use of relatively simplistic functional forms – linear, semilogarithmic and log-log forms being the norm" (Curry, Morgan & Silver, 2001). The primary exception to this observation is the use of Box-Cox models (Box, G. & Cox, D, 1964). More general nonparametric regression techniques, such as additivity and variance stabilizing transformations (Tibshirani, 1988), have seen little use. Reasons often given for not using non-linear forms include multicollinearity, reduced precision, and possible bias when used for prediction (Cassel & Mendelsohn, 1985). A recent attempt to overcome the problems of multicollinearity, posed by hedonic regression studies, and interpretation, posed by principal components analysis (PCA), is Arguea and Hsiao's (2000) use of Belsley's (1991) conditioning diagnostics to derive a simple set of predictors.

Psychometrics

Psychology specializes in descriptive theories of individual processes. Preference formation, liking, categorization, similarity, quantal choice and random utility theory are all in the domain of psychometrics. While areas such as experimental economics have appropriated many of the tools of psychologists, traditional economics is limited to supply and demand observations in the market place. (Experimentally measured indifference curves, mentioned earlier in efficiency frontier models, fall outside the market place. Their use was pioneered by the psychologist Thurstone (1931).)

With respect to hedonics, while almost all quantitative theories of decision making in psychology are based upon the concept of subjective expected utility, there is "no simple and general model for describing how preferences of individuals are determined and how choices are arrived at" (Kleindorfer, Kunreuther & Schoemaker, 1993). Some psychometric methods, such as biplots and vector models (Borg & Groenen, 1997), have the same non-negative marginal utility property as econometric models and should generally be avoided in sensory research unless the analysis is restricted to product benefits, *e.g.:* good taste, health, and value.

De Soete, Feger and Klauer (1989) note that "historically, two of the most important contributions to psychological choice modeling are undoubtedly Thurstone's (1927) law of comparative judgment and Coombs' (1950, 1964) unfolding theory."

These models, which account for satiety and allow negative marginal utility, may be used in univariate and multivariate contexts. Our attention here will be on the multivariate versions.

In their simplest form, unfolding models start with consumers' hedonic liking ratings for real products and estimate coordinates in a multidimensional space to represent both these real products and imaginary ideal products. Coordinates are estimated so that the resulting distances between an ideal product and the real products inversely approximate the hedonic evaluations – large distances indicate high disutility or low liking. Satiety is thus accounted for. For a dimension such as sweetness, a real product which is below the ideal product will be not sweet enough and a real product which is above the ideal product will be too sweet. If an attribute like "off-taste" is present, one where less is always better, then the ideal product should be located at the boundary of the space. Unfortunately, the empirical success of unfolding models does not always match their conceptual appeal.

A commonly used unfolding model in sensory analysis is Carroll and Chang's (Carroll, 1972) PREFMAP program (Greenhoff & MacFie, 1999; McEwan, 1996; Vigneau & Qannari, 2002). Output from a PREFMAP analysis of liking ratings for 13 berry flavored fruit drinks from 100 consumers and product profiles on ten attributes for the same 13 drinks from 25 assessors is shown in Fig. 2. The ten attributes of the study were color, aroma, cloudy, grape flavor, sweetness, tartness, naturalness, thickness, smoothness and aftertaste. A PCA of the mean product profile scores provided the location estimates of fruit drinks **a** through **m**. Dimension z_1 has very significant ($p < 0.01$) negative correlations with the attributes cloudy, aroma, grape flavor, tartness and a significant positive correlation with smoothness. Dimension z_2 has a significant ($p < 0.05$) negative correlation with sweet and a significant positive correlation with natural. Z_1 will thus be referred to as a weakness dimension and dimension z_2 will be referred to as a dietetic dimension. The symbols +, -, * and & indicate which dimensions are ideal or anti-ideal for each of the 100 consumers. (An anti-ideal dimension is one where utility *increases* with distance from the anti-ideal object.)

(Please insert Fig. 2 about here.)

While a cursory analysis of the PREFMAP output indicates that the program has performed satisfactorily, the median correlation of actual and estimated liking ratings for the 100 consumers was 0.91, further inspection results in a less optimistic conclusion. PREFMAP explicitly optimizes a squared error loss function. In its attempt to account for heterogeneity among consumers, it estimates (in the two dimensional case) five parameters for each subject – two for the location and three dimension weights (including a cross-product term) to indicate whether a dimension is to be interpreted as an ideal or anti-ideal dimension. (A nonmetric, quadratic model was estimated using PROC TRANSREG from SAS. It was chosen over other models because it possessed the best fit.) Overestimation is thus a very real danger. Since the number of estimates rises as the number of observations rises, the estimates cannot be said to possess consistency (Neyman & Scott, 1948). Furthermore, PREFMAP's estimates are derived from a polynomial regression analysis which introduces serious multicollinearity problems.

An evaluative measure other than the squared error loss function of PREFMAP is desirable for two reasons: (1) evaluations based upon the optimization criteria used by overestimated models are misleading, and (2) least squares criteria cannot be easily compared to criteria of other models that do not use least squares estimation. A simple intuitive measure that is not directly based upon the optimization measure and which does allow cross model comparisons is the correlation of actual first choices and estimated first choices, aggregated across all consumers. The ability, in the aggregate, to predict first choices should be a minimum criterion for any hedonic model. For PREFMAP, the correlation of the 13 element actual choice vector and the 13 element estimated first choice vector is 0.58.

Conceptual and structural limitations of PREFMAP are, however, of more importance than its statistical limitations. The model accounts for consumer heterogeneity but it does not account for inconsistency of judgments within consumers. The stimuli used in sensory studies can be very difficult to judge: they are usually unidentified, subjects are often not able to use their most powerful sense – sight, stimulus and neural events cause perceptual noise (Ennis, 2005) which can vary from object to object, and each consumer's ideal is also subject to moment by moment variation. A second limitation is the concept of an anti-ideal which can fluctuate from dimension to dimension. The seemingly random distribution of ideals and anti-ideals in Fig. 2 suggests that the distinction may be no more than another artifact of overestimation.

A probabilistic unfolding model that overcomes many of the limitations noted above is PROSCAL (MacKay, 2001; MacKay, Easley & Zinnes, 1995; http://www.proscal.com). PROSCAL brings together the unfolding model of Coombs and the comparative judgment model of Thurstone by assuming that real and ideal sensory objects are best represented as distributions, not points. More specifically, it is assumed that the sensory objects are normally perturbed and that it is through the variance attending the real and ideal sensory objects that variability enters the judgment process. Percept variance may differ from dimension to dimension and object to object. These assumptions distinguish PROSCAL from deterministic models which only make use of probabilistic concepts, if at all, in the process of fitting the model to the data to account for discrepancies between the data and the estimates of the model.

Unlike the least-squares regression procedure used by PREFMAP, PROSCAL uses an alternating maximum likelihood (ML) approach that employs a grid search procedure to sequentially reestimate variances, centroids and response model parameters. Response model parameters are the coefficients of linear exponential functions that relate the subjects' judgments to the underlying latent distances. Models of varying complexity can be compared by specifying equality constraints among variance parameters and among centroid parameters. Model comparisons are tested using Bozdogan's (1987) CAIC criterion.

Another significant difference between PREFMAP and PROSCAL is that PROSCAL has the ability to simultaneously estimate the parameters of the real and ideal objects from the profile data of assessors and the hedonic data of consumers. It can also test whether the two sets of data are compatible – can they reside in a common space? If the data cannot reside in a common space, then the hedonic data must be analyzed by themselves. CAIC is also used for common space tests (MacKay, 2005).

A final distinction is that while PROSCAL can estimate ideal distributions for individual consumers, it is really designed to estimate ideal distributions for consumer segments. By investigating segments, the consistency problems of PREFMAP are overcome. PROSCAL provides the option of using mixture models (McLachlan and

Peel, 2000) to assign subjects to segments. Segment models also provide interpretive advantages when it comes to analyzing market structure and evaluating new product possibilities.

The PROSCAL common space solution for the beverage data is shown in Fig. 3. Letters designate the thirteen real beverage centroids and numbers designate the centroids of the ideal beverages for the five segments identified by the program. The percentages of subjects represented by the five segments are 13%, 48%, 20%, 15% and 4%. Ellipses indicate the magnitude of the percepts' standard deviations. To enhance clarity, only unique ellipses are drawn.

(Please insert Fig. 3 about here.)

The large magnitudes of the standard deviations indicate a high degree of uncertainty among subjects in their evaluations of both the real and ideal products. Keeping the "weakness" and "dietetic" dimensional definitions used with the PCA and PREFMAP analyses, it is seen that the subjects are more sensitive to sweetness than strength when evaluating their ideal products. Products *k* and *m*, which are the two dietetic products, are more uniformly perceived on the dietetic dimension than on the weakness dimension. Similarly, product *d*, which has the highest score on weakness, is more uniformly perceived on the weakness dimension than the dietetic dimension. Overall, subjects prefer products with strong flavors and moderate sugar content. The one exception is subjects in the first segment who have a strong preference for dietetic products.

The advantage of the probabilistic PROSCAL model over the deterministic PREFMAP model is readily apparent when looking at the correlation of predicted and actual first choices. PROSCAL's correlation was 0.94, compared to 0.58 for PREFMAP. PROSCAL required only 48 parameters (36 location parameters and 12 variance parameters) while PREFMAP required 526 (226 location parameters and 300 dimension weights).

Hypothesis tests using the CAIC statistic (not shown) indicated that the common space solution of PROSCAL was appropriate. Comparisons (also not shown) were made of PROSCAL to another deterministic unfolding program, ALSCAL, and to a different probabilistic program, MULTISCALE. The performances of ALSCAL and MULTISCALE at estimating first choices were worse than PREFMAP.

Chemometrics

As the youngest of the three disciplines, chemometrics' tools have generally been borrowed from other areas. Partial least squares regression (PLS), developed by an econometrician, is the tool which chemometrics has come the closest to making its own.

Applied to hedonic analysis, a typical PLS application will model an n product by m variable response matrix $\mathbf{Y}$ of hedonic judgments as a linear function of an n product by p variable predictor matrix $\mathbf{X}$. Individual consumers, consumer segments or the average consumer ($m = 1$) can define the columns of $\mathbf{Y}$. The columns of $\mathbf{X}$ typically represent sensory and/or instrumental variables. Columns of $\mathbf{Y}$ and $\mathbf{X}$ are centered and usually standardized before beginning the iterative estimation process. To account for nonlinearities, quadratic terms may be included in $\mathbf{X}$.

PLS works by extracting successive linear combinations of the predictor variables and the response variables with the joint goals of explaining the response variation in $\mathbf{Y}$ and explaining the predictor variation in $\mathbf{X}$. The resulting latent vectors overcome the identification and multicollinearity problems that characterize multiple linear regression methods. A variety of algorithms for the latent space regression of **Y** on **X** is available. (PLS is a rapidly evolving area; the January 2005 issue of *Computational Statistics & Data Analysis* was devoted to PLS.)

The data evaluated with PREFMAP and PROSCAL were next evaluated using PROC PLS from SAS. Using default settings, the first analysis extracted the maximum number of factors, ten, and calculated the correlation of actual and predicted first choices for individual consumers as was done with PREFMAP. The resulting correlation, 0.77, compares much more favorably with PROSCAL than does the correlation obtained with PREFMAP. Unlike PREFMAP and PROSCAL, there is no global least squares or maximum likelihood criterion for PLS. It is, though, meaningful to compare the methods in terms of the number of parameters that are estimated. With ten predictor variables and 100 subjects, 110 partial regression coefficients are estimated per factor by PLS. (Estimates used in the standardization process have not been included.)

A large number of PLS models were evaluated. In terms of our first choice correlation criterion the best model, with a correlation of 0.87, was the one that was most like PROSCAL. Specifically, the model extracted two factors, used five segment response variables (instead of 100 individual response variables) that were assigned the mean responses of the subjects in the PROSCAL segments, added 45 quadratic predictor variables to account for satiety, and estimated the probability $\hat{P}_{ij}$ of choosing product *i* for segment *j* as the relative estimated response score $\hat{Y}_{ij} / \sum_i \hat{Y}_{ij}$. The final estimate $\hat{P}_i$ was simply the sample size weighted average of the probabilities for the five segments.

(Please insert Fig. 4 about here.)

Results of the two factor PLS model are shown in Fig. 4. The letters represent the **X** scores of the 13 products and the numbers represent the **Y** loadings (correlations) of the five segments. Comparison with the PROSCAL results of Fig. 3 is instructive. The configurations of the real products are somewhat similar for both models, the correlation of the 78 inter-point distances in the two models being 0.73. One difference in the configurations of the real products is that there is more "clumping" of the points in the PROSCAL solution. The clumping of the centroids occurs because PROSCAL is able to explicitly account for object variability. PLS cannot and unaccounted for variability has the artifactual effect of making the objects spread out (MacKay & O'Mahony, 2002). The second distinctive difference is that with PLS, the points representing the five response segments are in an arc in the second quadrant, indicating that all segments favor products with low to moderate values of z_1 and moderate to high values of z_2. No segments prefer moderate values of both characteristics. The PROSCAL story is a bit different. Segments 4 and 5, for example, are said to prefer objects with average values of z_1 and z_2. A summary comparison of the primary methods evaluated is provided in Table 1.

(Please insert Table 1 about here.)

Conclusion

Probabilistic multidimensional scaling (PMDS) and PLS are methods that offer insights to the analyst. ML PMDS has a rich base in probability theory and offers the advantages of hypothesis testing in model selection (MacKay and Lilly, 2004). We find the ideal point interpretation of PMDS very appealing and have elsewhere (MacKay,

2005) noted the ease with which “perceptual shares” for new products may be estimated and optimal products designed. The PMDS unfolding output is also easy to convey to marketing managers and can be readily used for making strategic product development decisions. PLS offers the ability to accommodate massive numbers of independent variables, a common occurrence with instrumental data, and to do cross validation. The spread of PLS development beyond chemometrics should provide additional benefits to users in the sensory sciences.

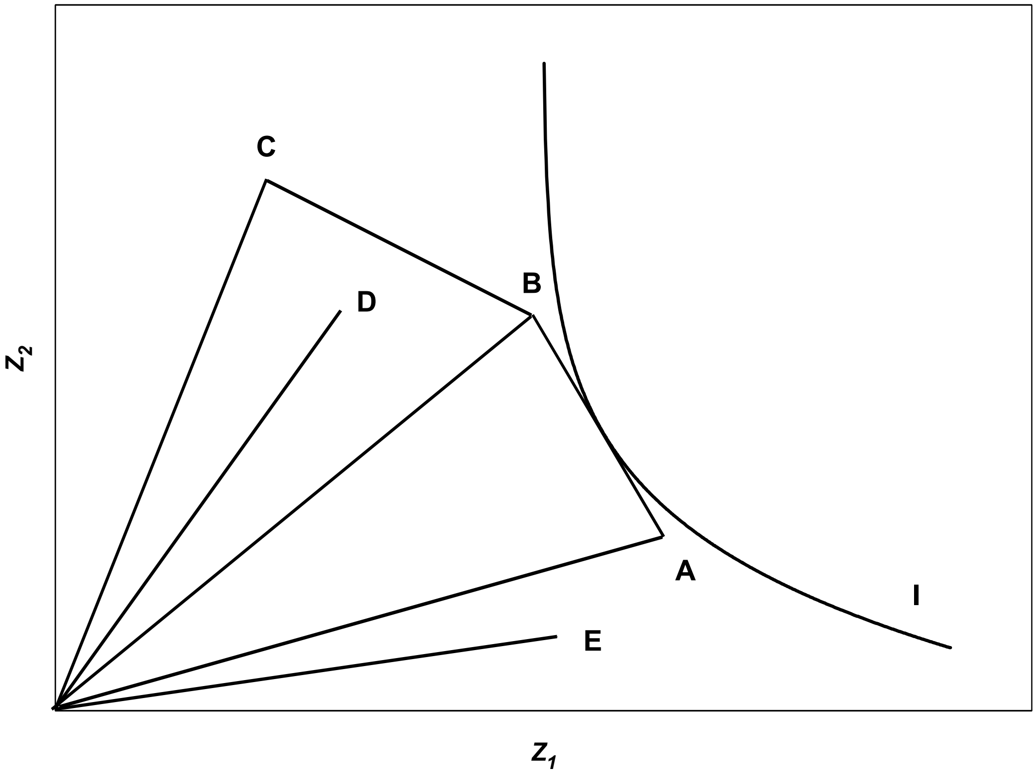
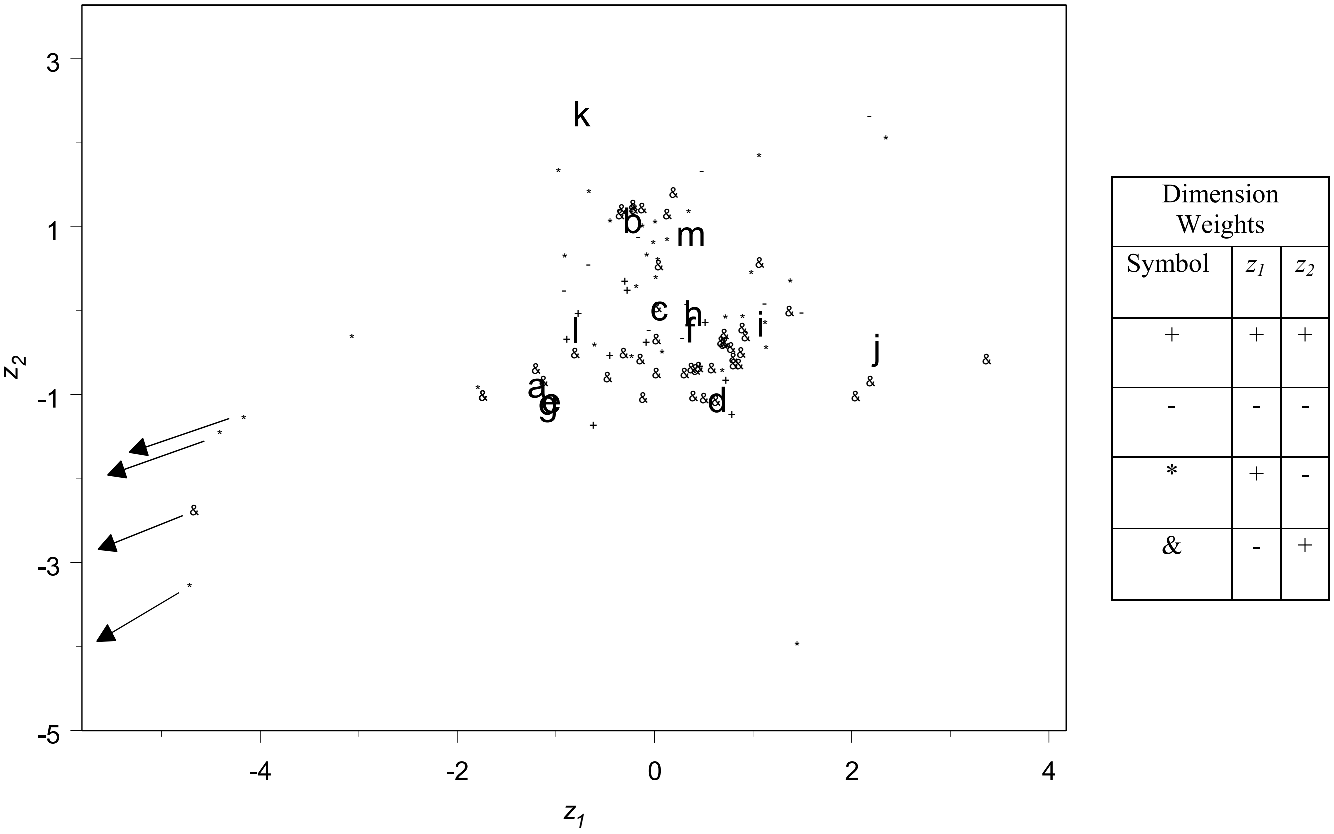


Fig. 1. Indifference curve and the efficiency frontier



Dimension Weights		
Symbol	z_1	z_2
+	+	+
-	-	-
*	+	-
&	-	+

Fig. 2 Deterministic unfolding solution from Prefmap.

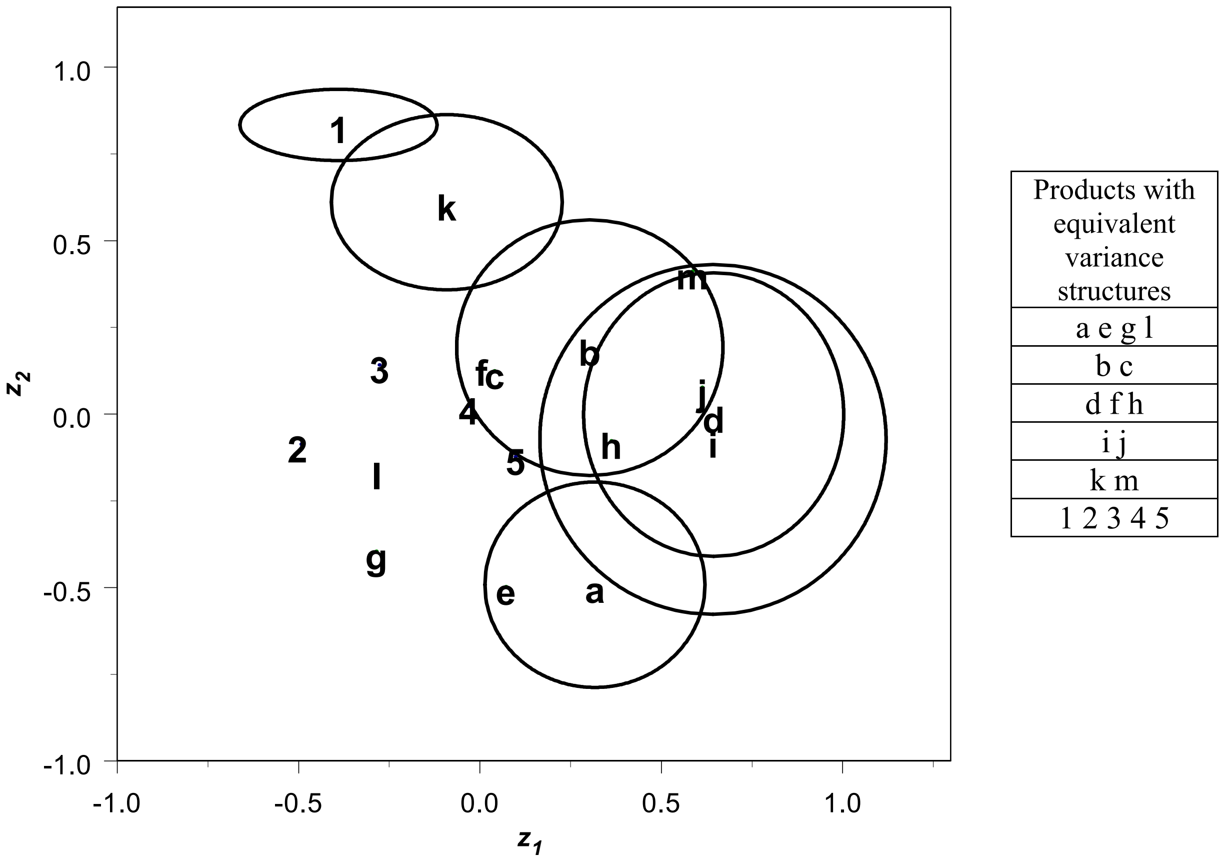


Fig. 3 Probabilistic unfolding solution from PROSCAL. Standard deviational ellipsoids for some objects have been omitted for clarity. See the text for the assignment of objects to ellipsoids.

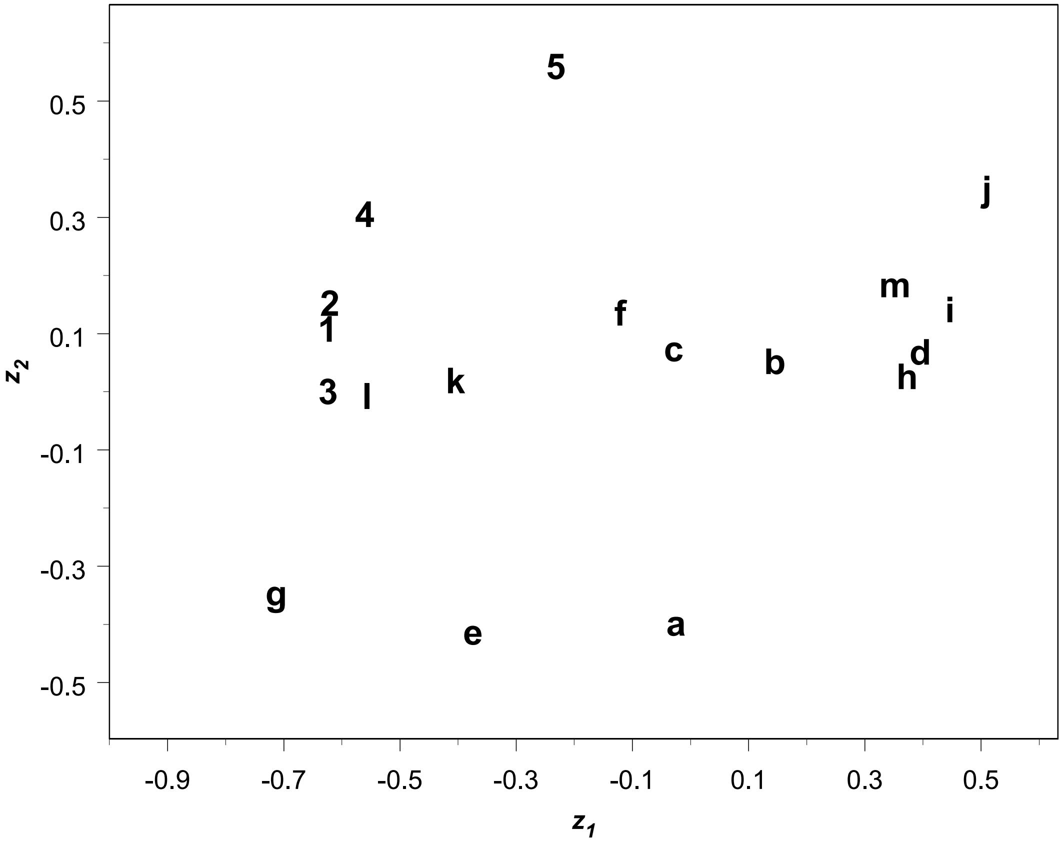


Fig 4. PLS solution using PROSCAL groups.

TABLE 1. Performance of Methods

Model	Correlation of Predicted and Actual First Choices	Number of Estimated Parameters
PREFMAP	0.58	526
PROSCAL	0.94	48
PLS – ten factors	0.77	1100
PLS – two factors[1]	0.87	120

[1] See text for full description.

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