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Combination Rules for Judgments of Odor Quality Difference

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Observers judged the similarity of odorants to seven descriptor words (ethereal, camphoraceous, musky, floral, pepperminty, pungent, repulsive), and also judged the direct dissimilarity of pairs of odorants to each other. The method of multiple linear regression analysis was used to yield a predictor equation relating overall dissimilarity of odorant pairs D_{ij} to their absolute differences on each of the seven profile components (d_{ij}): $D_{ij} = k_1 d_{ij1} + k_2 d_{ij2} \ldots k_7 d_{ij7}$. The values $k_1 \ldots k_7$ were not equal to each other in the regression equation, indicating that in the prediction of subjective quality differences some attributes take on more weight than others. As k_i increases, dimension i (an attribute) becomes increasingly salient in perception. When odors are represented as points in a subjective geometry of quality, distances between odorants cannot be computed by standard distance formulas, since some dimensions in the geometry are expanded, whereas others are contracted.

Sensory studies of odor quality have produced a proliferation of methods for representing odor quality in terms of a geometrical space of relatively low (1–3) dimensionality. With the advent of high-speed computers the analysis of subjective responses to odors has greatly expanded, as increasingly complex forms of data analysis and reduction have become feasible and easily available to the researcher. The present paper focuses upon a technique called "salience analysis," which determines how the human judge weights various quality attributes of an odor in order to decide how dissimilar pairs of odorants appear to be from each other. The procedure is a variety of data analysis designed for post-experimental (off-line) use, although with appropriate modifications it may well become useful for on-line monitoring of organoleptic evaluation of odors.

Numerous approaches to a classification of odor qualities have been proposed and reviewed extensively (Harper *et al.*, 1968a). Odor classification can be as simple as the selection of four basic descriptors (fragrant, acid, burnt, caprylic; Crocker and Henderson, 1927), or as complex as a list of several hundred words selected from the available descriptors in the dictionary. A recent list comprised 44 such descriptor terms culled from a much larger list (Harper *et al.*, 1968b; Harper, 1974). For specific applications the 44 general terms may not be sufficiently inclusive, and other and more specific terms must be used. The descriptor list becomes, therefore, a fluid entity, changing shape and constitution to fit the needs of the experiments in which it is used. Finally, there exist other descriptor systems, such as the series of seven proposed by Amoore under the rubric of the Stereochemical Theory of Olfaction (Amoore and Venstrom, 1966). These descriptors (ethereal, musky, camphoraceous, pepperminty, floral, pungent, and putrid) are assumed either to correspond to differently shaped receptor sites on the olfactory mucosa (descriptors 1–5) or to electrical charges on the molecules (*viz.*, pungent and putrid).

Another approach to odor quality is called "multidimensional scaling" or "proximities analysis." The approach attempts to place odorants into a geometrical space of some defined and low dimensionality (usually 3 or fewer). The rules for placement are straightforward—odorants that are qualitatively dissimilar are separated from each other in the space by large distances whereas odorants that are similar are separated by small distances. A number of algorithms exist by which human subjective judgments of odor similarity or dissimilarity are first converted to interpoint distances, and these distances are processed to evolve a geometrical space. The interpoint distances in the space may be monotonically related to or even linearly related to the dissimilarities judgments (Shepard, 1962; Torgerson, 1965; Kruskal and Carmone, 1969).

The axes of the geometrical space that are developed from proximities analysis are useful, both in terms of a shorthand representation of where odorants lie (*i.e.*, a dictionary of odors as points in space) and in terms of the potential discovery of "primary" orthogonal psychological dimensions of odor perception. Typically, the first axis to be developed in the space is that of pleasantness–unpleasantness, corresponding to the primary dimension along which judgments of dissimilarity are made. The remaining axes of the space depend critically upon the initial selection of test odorants, their number, and their salient characteristics. When a small sample is selected, then the geometrical space will be considerably sparser than when a larger number of chemicals are evaluated.

The present study combines profile analysis of odorants with proximities or dissimilarities analysis. Its principle aim is to determine how the overall dissimilarity of odorants is predicted from differences of odorants along corresponding attributes of a quality profile. In equation form, the model to be tested is expressed by the simple linear equation

$$D_{ij} = k_1 d_{ija} + k_2 d_{ijb} \ldots k_n d_{ijn} \qquad (1)$$

According to eq 1, D_{ij} refers to the overall estimate of the dissimilarity (subjectively estimated) and without specific instructions about which attributes should be considered. The values $d_{ija} \ldots d_{ijn}$ refer to the absolute differences between two odorants (ij) along a series of dimensions (or profile attributes) $a, b, \ldots n$. These are obtained indirectly, by comparing two profiles. Finally, the coefficients $k_1 \ldots k_n$ refer to weighting factors that transform the absolute distances to dissimilarity values. The model assumes that overall dissimilarity between odorants (in olfactory quality) is a weighted sum of their component differences.

One of the useful outcomes of this approach is its ability to describe either stimuli or individuals according to the values $k_1 \ldots k_n$ that they generate in the profile and dissimilarities tasks. Another outcome is the refinement of profile procedures to include only attributes that have high salience values (*i.e.*, high levels for the coefficients in the salience equation, 1).

EXPERIMENTAL PROCEDURE

The experimental portion of the study was divided into three sections: evaluation of various odorants at different concentrations to yield stimuli of equal odorous intensity,

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evaluation of odorants at three intensity levels along a profile of seven attributes by an organoleptic procedure, and evaluation of the apparent dissimilarity in odor quality between pairs of chemical odorants. The stimuli were reagent grade chemicals (except when noted), diluted in odorless benzyl benzoate (Eastman Organic Chemicals). All odorants possessed their characteristic notes, indicating relative sensory purity. The odorants were: (1) methyl salicylate (wintergreen, J. T. Baker, Inc.); (2) eugenol (oil of cloves, J. T. Baker); (3) benzaldehyde (almond-like, J. T. Baker); (4) 1-propanol (rubbing alcohol, ethereal, J. T. Baker); (5) ethyl cinnamate (cinnamon, spicy, sweet, J. T. Baker); (6) guaiacol (burnt, smoky, J. T. Baker, Practical grade); (7) thymol (camphoraceous, medicinal, Sigma Chemical Co.); (8) anethole (anise, licorice, J. T. Baker); (9) citral (lemon, citrus, J. T. Baker, practical grade). The odorants possessed different chemical structures, and spanned a wide range of organoleptic qualities and hedonic tones. The odorants were diluted in 4:1 (by volume) ratios in benzyl benzoate (except thymol, which was diluted in 2:1 volumes in distilled and deionized water). Initially, five levels of each substance were prepared (4^0, 4^{-1}, 4^{-2}, 4^{-3}, 4^{-4}) to yield a wide range of nominal physical concentrations. From these five levels equally strong (organoleptically) odorants were selected for the subsequent experiments.

The odorants were presented to the panelists in small test tubes. Each odorant in its solvent was maintained in the test tubes. A glass rod protruded from an aluminum foil covered cork, and extended into the stimulus liquid (approximately 3 cm^3 at the base of the test tube). Glass wool was wrapped tightly about the base of the glass rod, and was immersed in the liquid at all times except just prior to and during sensory evaluation. In order to take a sample sniff the panelist simply uncorked the test tube, pulled the cork and glass rod slightly, shook the rod against the side of the test tube to dislodge any liquid, and removed the cork and glass rod to smell the tip of the wick. Although the precise measurement of odorant concentration cannot be specified for the "cloud" of odorant, the procedure sufficed for the qualitative dissimilarity judgments, and for estimates of different odor intensities. The procedure appeared adequately reproducible, and the panelists were instructed to maintain a standard way of sniffing the wick.

The panelists first judged the apparent odor intensity of all odorants by the method of magnitude estimation, in which their numerical estimates reflect ratios of odor intensity. Ratios on the subjective scale were to correspond to ratios of odor intensity. Citral at 100% was used as the standard, and called "10," and the panelist rated all other odorants in proportion to the intensity of the citral standard. An estimate of 1, for example, means that the odor strength is only 10% as strong as that of citral. This procedure was used to determine physical concentrations (in liquid dilution) that produced magnitude estimates of 10, 7, and 3, respectively. The following odorants produced the requisite odor strengths: level 10, guaiacol, ($1/16$), citral (1), propanol ($1/64$), benzaldehyde ($1/16$), eugenol ($1/16$), methyl salicylate (1); level 7, guaiacol, ($1/256$), citral, ($1/4$), benzaldehyde ($1/256$), eugenol ($1/64$), methyl salicylate ($1/16$), anethole ($1/64$); level 3, thymol ($1/4$), propanol ($1/256$), eugenol ($1/256$), ethyl cinnamate ($1/4$).

In experiment I a group of 12 scientists and engineers at the U. S. Army Natick Laboratories (10 males, 2 females, ages 18–35) rated each of the compounds listed above along a profile of seven descriptor attributes (ethereal, camphoraceous, musky, floral, pepperminty, pungent, repulsive). These are the seven odor classes proposed by the Stereochemical Theory (Amoore and Venstrom, 1966). Each panelist rated the odorants in terms of how appropriate each descriptor appeared to be. They used a six-point category scale (0 = inappropriate or not present in the odor, 5 = very appropriate and strong in the odor). The panelists paced themselves and were permitted to evaluate each odorant as frequently as desired. As in the evaluation of odor intensity of the larger set the panelist sniffed the odorant from the glass wool wick attached to the glass rod. In order to prevent fatigue, however, each panelist was required to wait at least 10 sec between samples. The panelists were untrained in both profiling and in the method of quality dissimilarity estimation. No reference chemicals were provided to the panelists, who were instructed to rely upon what they thought best represented their own individual concepts of camphoraceous, minty, etc.

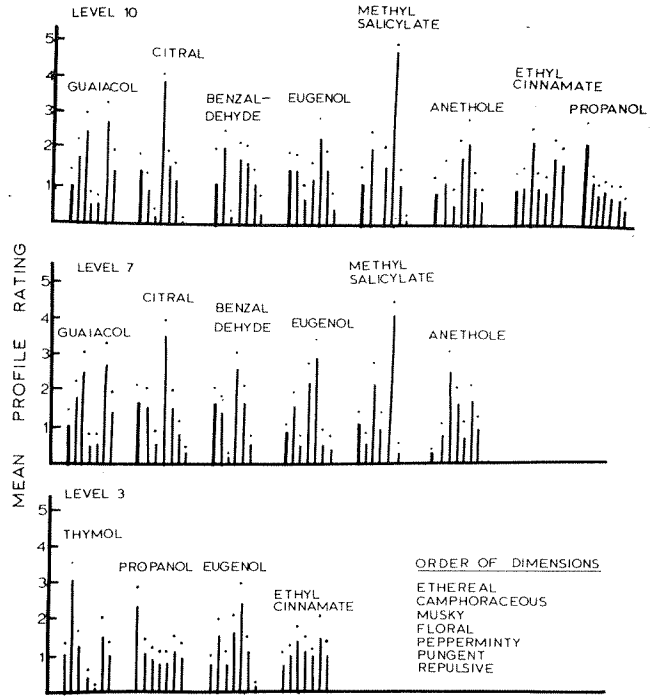

Figure 1. Odor profiles for odorants evaluated in the present experiment. The profiles represent averages of 12 observations. Points above each profile value are the rating + 1 standard error and provide confidence limits for the profiles.

RESULTS AND DISCUSSION

Figure 1 shows the profiles for the odorants, as well as the value corresponding to the mean rating + 1 standard error. Each odor possesses its characteristic profile, which may change somewhat upon increased odorous intensity. For example, thymol possesses a marked camphoraceous character, whereas methyl salicylate is predominantly minty. Other side notes appear in each odor, as indicated by Figure 1. When the overall intensity of the odorant is raised only methyl salicylate (oil of wintergreen) possesses a sufficiently characteristic odor so that its minty note approaches the maximum value of 5. The remaining odors have ratings distributed among the different descriptor adjectives. In general, odorants at low and moderate intensities tend to have more peaks in their profile of commensurate height, suggesting either that the odorants become more complex at lower levels, or that their odor qualities at these low levels are relatively indistinct and fuzzy. As odorants increase in intensity their profiles sharpen, so that fewer major peaks stand out above the other descriptors.

In experiment II the aim was to determine a measure of subjective dissimilarity between pairs of odorants. The ultimate aim was to provide a useful dissimilarity measure that would be eventually related to the dissimilarity of pairs of odorants in terms of their respective quality

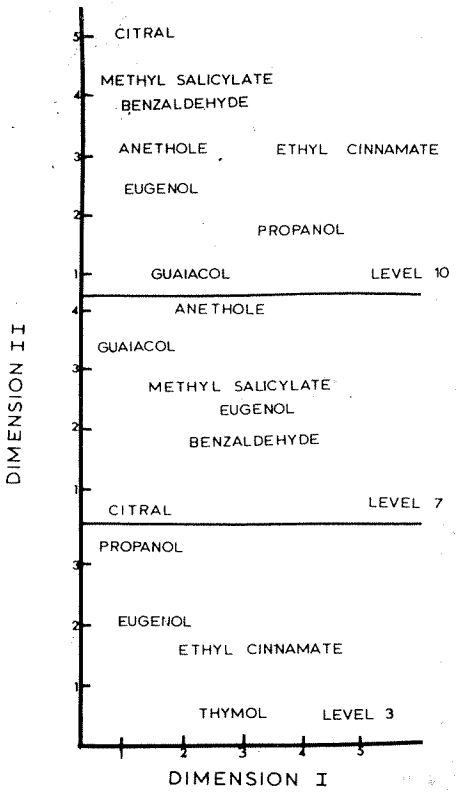

Figure 2. Two-dimensional geometrical spaces for the three levels of odorant intensity. Each odorant is located as a point in this two-dimensional space. Odorants that are far from each other are those that are qualitatively dissimilar by direct judgment.

profiles. As such, experiment II provided complementary information to the profile procedure and permitted the correlation of two types of organoleptic judgments.

The same panelists participated in experiment II as has had in experiment I, and the stimuli were also the same. Each panelist was instructed to judge the dissimilarity between selected pairs of odorants using a scale from 0 (identical) to 1.0 (absolutely different or maximally dissimilar). The pairs were selected to remain within a single intensity level. Thus, at level 3 there were $4 \times 3/2 = 6$ pairs, at level 7 there were $6 \times 5/2 = 15$ pairs, and at level 10, $8 \times 7/2 = 28$ pairs. Each panelist thus made a total of 49 judgments of overall dissimilarity between odorant pairs. The order of pairs was randomized, and the order of odorants within each pair was also randomized.

Odor dissimilarity judgments can be treated as if they are distances between odorants. Figure 2 shows one possible geometrical space for the three intensity levels of the odorants. The geometrical spaces were obtained by the computer program MDSCAL 5M, which was instructed to determine only a two-dimensional configuration. With increasing dimensionality the goodness-of-fit of the geometry increases, so that the correlation between interpoint distances in the space and originally estimated dissimilarities approaches 1.0 (perfect agreement). The points cluster into two groups; one group appears to be odorants that are best characterized as sweet, fragrant, flowery, and typically pleasant, whereas the other group (or groups) is idiosyncratic in nature, and not easily identified.

Salience Analysis. Profiles of several qualitative attributes and estimates or odor dissimilarity are two aspects of the subjective judgment of odors. The former is an index of the sensory constitution of the odor whereas the latter is an integrated judgment that, presumably, is based upon several aspects of the profile.

Table I. Parameters of the Salience Equations

(I) Summation of linear differences

$$D_{ij} = 0.53(d_1) + 0.33(d_2) + 0.45(d_3) + 0.56(d_4) + 0.22(d_5) + 0.18(d_6) - 0.33(d_7)$$

(standard error of the regression = 0.12)

(II) Summation of squared differences

$$D_{ij}^2 = 0.87(d_1^2) + 0.89(d_2^2) + 0.85(d_3^2) + 0.90(d_4^2) + 0.27(d_5^2) + 0.40(d_6^2) - 1.24(d_7^2)$$

(standard error of the regression = 0.15)

(III) Summation of cubed differences

$$D_{ij}^3 = 1.09(d_1^3) + 1.90(d_2^3) + 1.43(d_3^3) + 1.25 \cdot (d_4^3) + 0.31(d_5^3) + 0.74(d_6^3) - 3.63(d_7^3)$$

(standard error of the regression = 0.15)

(IV) Summation of linear differences with additive constant

$$D_{ij} = 0.04(d_1) - 0.11(d_2) + 0.29(d_3) + 0.29(d_4) + 0.07(d_5) + 0.13(d_6) - 0.16(d_7) + 0.43$$

(standard error of the regression = 0.10)

(V) Summation of squared differences with additive constant

$$D_{ij}^2 = -0.04(d_1^2) - 0.14(d_2^2) + 0.41(d_4^2) + 0.41(d_4^2) + 0.08(d_5^2) + 0.39(d_6^2) - 0.37(d_7^2) + 0.30$$

(standard error of the regression = 0.12)

(VI) Summation of cubed differences with additive constant

$$D_{ij}^3 = -0.40(d_1^3) - 0.16(d_2^3) + 0.48(d_3^3) + 0.53(d_4^3) + 0.09(d_5^3) + 0.83(d_6^3) - 0.66(d_7^3) + 0.21$$

(standard error of the regression = 0.12)

The present approach relates profiles to dissimilarities by the salience equation mentioned above. There are seven descriptors and therefore seven terms in the multiple linear regression equation. Equation 1 is only one of many possible predictor equations. Depending upon the conceptualization of the judgment process, eq 1 may be modified to predict the square of the dissimilarity judgment between two odors as a linear combination of their squared absolute differences on corresponding profile attributes. In eq 1, this would be represented by squaring each observation prior to solving for the least-squares coefficient. Equation 1 represents one type of combination rule for difference judgments known as the city-block metric. Its modification by the replacement with squared differences turns the combination rule into the standard Euclidean distance (squared). Finally, higher order multiples may be used in place of the linear or square values. Each power generates its own set of coefficients, and each corresponds to its own unique type of combination rule. In general, however, each of the powers falls into the class of metrics known as the Minkowski metrics, of which the city-block and the Euclidean distance varieties are simply the best known representatives. In addition, the additive constant k_8 can be left free to vary or may be constrained to equal 0. The latter case defines a function (*i.e.*, a hyperplane) that goes through the origin. It implies that when two profiles coincide, all component differences become 0, and the dissimilarity value becomes 0 as well.

Table I presents the least-squares estimates for the coefficients of the regression equations. Values for these coefficients were determined for three different powers of component differences (r = 1, 2, 3) and both for freely varying additive constants and constants constrained to equal 0. The standard error of the regression is also presented as an index of the goodness-of-fit. The standard error represents the variation of the points around the line (or plane) of best fit.

As a first approximation the coefficients of the salience equation are unequal to each other, so that some attributes are more important than others in the prediction of overall quality differences. Differences in the "floral" character and in the "ethereal" character of odors tend to be most important in differentiating odors, when the

function for salience is computed without an additive constant. Differences in the floral and in the muskiness of odors tend to be most important when the salience function is computed with an additive constant.

The exploration of different exponents for absolute differences (linear, squared, and cubed values) suggests that the absolute values of the coefficients in the equations change, according to the power selected, but that their monotonic order tends to remain approximately constant. In addition, asymptotically, the elimination of a constant term in the salience function tends not to influence the goodness-of-fit to any substantial degree. However, with fewer predictors than the full complement of seven, the constant term in the equation produces increasingly better prediction relative to the same equation, but without the constant term. This phenomenon means that with increasing numbers of predictor attributes in the salience equation more and more of the judged differences between odors can be accounted for by appeal to the differences of these odors along the profile.

In the present results a number of points should be noted before attaching undue significance either to the form of the function used or to the values of the parameters that indicate relative salience. First, only seven descriptors out of a possible several hundred were used here, so that the salience equation is incomplete. In addition, only nine odorants were used, out of several thousand possible ones, so that the coefficients for the equations are based only upon a limited sample of compounds that evoke olfactory impressions.

The present approach of salience analysis provides a simple, easily implemented procedure for assessing the importance of odor descriptors in the characterization of odor perception. The model is straightforward, and the computational mathematics are already feasible, and available in already developed "canned programs." Conceptually, the approach permits the flavor investigator to quantify the relative importance of descriptors, but also allows him to quantify the panelists as well. Rather than averaging the judgments of the 12 panelists (or as many as participate in the study), the experimenter may choose to obtain several replicate judgments from each panelist, and produce salience functions for each panelist. These functions provide a signature of each panelist, for they indicate the degree of importance that he places on each of the attributes in the profile of descriptors. In addition, pairs of odors can be studied if a sufficiently large group of panelists judge the pair, both by profiling and for qualitative dissimilarity. In the analysis of odor pairs, care must be taken to remember that the salience equation represents a sample of cross-sectional information, so that the variation among panelists (not among stimulus odorants) provides the needed information with which to obtain the coefficients.

Although salience analysis is designed with the purpose of mapping an individual's perception of the odor world about him, it may well have uses for correlating subjective and instrumental responses to flavors. A profile might be the various peaks from a gas chromatographic analysis of one flavor. For several such gas chromatographic analyses, both difference spectra (instrumentally assessed) and subjective estimates of dissimilarity might be obtained and subjected to the analysis discussed above. The result would be the relative importance of differences in peaks that contribute to the differences, organoleptically evaluated.

A final word is in order about the relation of this approach to other, similar approaches such as discriminant analysis. Salience analysis is founded upon the premise that the pairs of odorants being compared vary in dissimilarity. No requirement is made that these odorants be classified into separate groups, and, in fact, the analysis is based upon the differentiation of odorants along a continuum. Discriminant analysis, in contrast, requires that the odorants be placed into different groups entirely by a classification procedure. Hence, the two analyses complement each other, and each provides its own approach into the computerized analysis of flavors. Discriminant analysis is more appropriate when the categorizations of flavor are already decided, whereas salience analysis has the interesting and perhaps useful possibility of indicating the expected dissimilarity between pairs of flavors (odors, etc.) when one of the flavors is modified slightly, and its profile altered.

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