Psychological Qualities of Odor II: Geometry of Odor Quality

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Multidimensional scaling is the general term for the set of approaches which share the aim of inserting odor stimuli, as points, into a geometrical space of low dimensionality (2-3 dimensions).

The properties of this space and of the points (which are the odors) are as follows:

(a) Stimuli which are close together, in terms of distance from each other in the space, are those which are perceptually quite similar to each other. Conversely, stimuli which are far away from each other are those which are perceptually quite dissimilar.

(b) In order to arrive at the proper positioning of points in this space, empirical estimates of overall qualitative dissimilarity have to be made for points of odors. The panelist (novice or expert) sniffs pairs of odorants and assigns a number to reflect how different they smell. These numbers then reflect subjective estimates of dissimilarity. The matrix of data that emerges from the study is triangular. The columns represent the odors, the rows represent the odors, and the entries represent the judgment of how different in odor quality each pair of odorants seems to be.

Computer programs have been developed which work with the empirically estimated dissimilarities between odor pairs and reconstruct a geometrical space, so that the distances between odors in this space best accord with the judged dissimilarity between odors. Some of the programs, such as M-D-SCAL 5M (Kruskal and Carmone, 1969) account only for group results, so that the experimenter has to average the dissimilarities from a panel of individuals before reconstructing the space. Other computer programs have the ability to compute an overall odor geometry, and then compute individual weighting factors (INDSCAL, Carroll and Chang, 1969). The INDSCAL program which accounts for individual differences is based upon the working hypothesis that we share a general odor geometry, containing a few fundamental dimensions. However, each of us brings idiosyncratic stretching or shrinking factors to each dimension. We may notice differences on one dimension and ignore differences on another. Others may notice differences on both dimensions.

Methods for multidimensional scaling

There are three methods for developing multidimensional maps. One is the direct estimation of dissimilarity (or similarity) between pairs of odors. Occasionally, the experimenter may also want to use concepts and instruct the panelists to estimate the following:

- Dissimilarity between all pairs of odors.
- Dissimilarity between all pairs of word descriptors which are to take the role of ideal sensory aspects. For instance, how different is the concept of a woody aroma from the concept of a spicy aroma?
- Dissimilarity between all heterogeneous pairs, comprising an odor and a descriptor (Moskowitz and Gerbers, 1974).

The second method is to evaluate quality profiles of odorants in which the panelist has scaled the odorants on various attributes. Here the analysis is more of a content analysis—how different two odorants with a specific type of sensory profile are from two other odorants with different sensory profiles.

The methods used for estimating dissimilarity for profiling data are somewhat different than those used for dissimilarities data. One may consider the profile matrix to be a matrix of dissimilarities between odorants and descriptors. If in a matrix odorant A (limonene) is rated high on a specific descriptor term (citrus-like), then we assume that A and the descriptor term are similar to each other qualitatively. On the other hand, if odorant A is rated low on a descriptor (burnt, smoky), then we assume that A and the descriptor term are dissimilar to each other. Note that one can process this matrix of profile data as if it were a matrix of dissimilarities, wherein all elements from one set (odors) are compared to all elements of another set (descriptors). However, one never compares elements from the same set (odors to odors, descriptors to descriptors). The results of this analysis yield a geometrical space comprising what is called unfolded profiles. In the geometry of odor, both the descriptors and the odors are embedded in the same odor space.

The third method is the factor analysis procedure (Harman, 1966). Factor analysis consists of first determining the correlations, or the degree of relatedness, among a series of odorants, based upon how similar they are when rated on a set of descriptor attributes. The index of relatedness is the Pearson correlation coefficient. Odorants exhibiting similar or covarying descriptor profiles are highly correlated with each other. If odorant A is rated high on attribute 1 and low on attribute 2, and if odorant B is also rated high on attribute 1 and low on attribute 2, then they are correlated. Odorants exhibiting unrelated sensory profiles are uncorrelated with each other. The factor analysis method looks at the set of pairwise odor correlations (based upon their profiles), and assigns them to a location in a geometrical space. The axes of this space are then odor primaries. Note that either the odorants or the descriptor terms, respectively, can be factor analyzed.

The studies in the appendix utilized experiments in which the following variations have been made:

- Many different odors, or just a set of related odors, have been considered.
- Experimenters have asked panelists to estimate the perceived dissimilarity directly, or to profile the odors using a set of descriptor terms.
- Experimenters have processed the dissimilarity estimates by multidimensional scaling, *or* have factor analyzed the profiles, *or* have used the profile data for unfolding, *or* have used the profiles to construct an estimated geometrical distance between pairs of odors. (This distance can be obtained by lining up in parallel the profiles of two odorants, computing the difference on equivalent attributes by subtracting one profile from the other, squaring the difference, summing the squared differences, averaging, and then extracting the square root. The result is a single index number which corresponds to the geometrical distance between the odorants.)

Other uses of multidimensional scaling in odor perception

Moskowitz (1976) advocated a somewhat different approach to using the technique of multidimensional scaling to evaluate odor perception. The thesis of the argument was that by a selection of a representative group of odors, one could recover only a limited set of dimensions which would be specific to those odors. An evaluation of the entire spectrum of odors to insure total representation of all stimuli was not feasible. Instead, one should try to find out, through multidimensional scaling, how we psychologically combine various odorants. One could establish the dimensions before the experiment by selecting a representative series of odors, mixing these together in varying proportions and in different combinations, and then submitting the melange of odors (both mixed and unmixed) to a panel of judges who would not know which stimuli were simple odorants and which were mixtures.

In the published report using multidimensional scaling procedures, the results showed that the following phenomena occurred for the set of 5 odorants (total of 31 test odorants), mixed in combinations of 1, 2, 3, 4 and 5.

1. Simple, unmixed odors lay toward the outside of the two dimensional odor space. The five simple odors were methyl salicylate, oil of wintergreen (sweet), caproic acid (fatty, oily, goaty), isobutyl isobutyrate (fruity, estery), dimethyl disulfide (rotten, cabbage), and camphor (camphoraceous).

2. Mixtures lay in the middle of the two dimensional odor space so that one could conclude that the qualities of mixtures were intermediate to the qualities of their components. Mixtures of 4 and 5 components tended to lie closer to the middle of the space than did mixtures of 2 and 3 components.

3. In binary mixtures some odorants behaved as "dominators." In binary mixtures with other dominators, the quality of the mixture was quite dissimilar to either element alone. Methyl salicylate and methyl disulfide both acted as dominators. Other odorants (caproic acid and isobutyl isobutyrate) behaved in a less dominant way. A dominator mixed with one of these other odorants smelled quite similar to the dominator, so that the other quality was eliminated. However, a mixture of two nondominator odorants smelled intermediate between the two. Finally, camphor was dominated by the other four odorants.

The use of multidimensional scaling to evaluate quality shifts in odor mixtures may prove to be a fruitful approach because the investigator need not rely upon changes in physical/chemical properties to produce stimuli for the evaluation. Rather, experimenters can produce their own set of stimuli by mixing odorants at any derived relative concentrations. Also, the experimenter can learn about the laws of perception of odor quality. Is odor quality governed by a simple underlying algebra, or is a mathematical model of odor perception impossible to develop? One of the most important things about the mixture study was that one important property of algebra, transitivity, was found. If odorant A dominated odorant B (so the mixture smelled like A, not at all like B), and if odorant B dominated odorant C, then odorant A dominated odorant C. The multidimensional scaling method thus provides a picture of odor quality changes, as well as a geometric map on which one can compare the positions of simple odors and their combinations.

Overview of multidimensional scaling

The foregoing approaches and results illustrate the new wave of research on multidimensional representation of odor perception which continues to produce a spate of geometries of odor. Researchers should keep in mind the following questions when evaluating the information and importance of these geometrical representations.

- Is the geometry a general one, or does it reflect a narrow corridor of the odor space, due to the limited selection of odorants?
- Does the geometry provide insights other than a restatement of odorant dissimilarities?
- Does the geometry allow the experimenter to predict other aspects of behavior, in addition to dissimilarity? For instance, will similar odors be substitutable for each other in products?

As research on odor perception increases, we may well expect to see applications beyond the development of simple odor spaces. Mixture studies, especially, may be fruitfully evaluated using multidimensional scaling solutions simply as geometric representatives of the data. The experimenter may be able to derive insights from the pictorial representation. As in any other science, the methods developed in psychometrics to represent stimulus dissimilarity may in the long run prove more valuable as an aid to creative intuition than as direct answers to odor perception questions.

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Appendix

Yoshida–Experiment I (1964)

Odorants tested: Odorants selected to represent a collection of stimuli from theories of odor classification (Henning, Zwaardemaker, Crocker and Henderson)

Examples: Jasmin, vanillin, lemon, methyl mercaptan, caproic acid

Subject: Yoshida

Scaling: 10 point dissimilarity scale

Results: Three distinct dimensions emerged: I: Pleasantness/unpleasantness, II: Sweet—pungent, III: Trigeminal (pain, feeling)

Yoshida–Experiment II (1964)

Odorants tested: Same as in I (above)

Subjects: 5 female subjects naive about olfactory theory

Results: Four dimensions were extracted: Dimension IV: Odor intensity

Yoshida–Experiment III (1964)

Odorants tested: Odorants selected to represent Piesse's theory of perfumery (odorants were likened to keys of a musical scale). According to Piesse's theories, there exist octave-like relations among the odors (eg, almond, heliotropin and vanilla are in the same category).

Examples: Group I: Jasmin, camphor
Group 2: Bergamot, heliotropin, vanilla
Group 3: Acacia
Group 4: Musk
Group 5: Neroli
Group 6: Lavender, Peru balsam
Group 7: Menthol, cassia oil
(Odorants were presented at full strength, undiluted)

Subjects: One male and six females, each judged the similarity of each pair twice

Results: Four factors were found (but not named). In addition, odors of the same note should, but often do not, lie close to each other. There is no dimension which corresponds to tonality. There is no dimension which corresponds to the "pitch" of the note.

Yoshida–Experiment IV (1964)

Odorants tested: McCall's scheme of perfumes, which classifies perfumes according to user groups:
Single florals (White Rose, Jasmin, Heliotropin)
Floral Bouquet (Arpège, Paris, Amour Amour)
Modern Blends (Chanel No. 5, L'Aimant)
Oriental Blends (Emeraude, Shalimar, Tabu, L'Origan)
Woody-Mossy-Leafy (Soir de Paris, Mitsuko, Cypre)
Spicy Bouquet (Cappi)
Fruity Bouquet (Fleurs de Cocailles)

(These perfumes fall into distinct user groups. Groups 1 and 2 are suitable for young ladies, whereas groups 3-7 are suitable for mature women.)

Subjects: 25 females

Scaling: Each perfume on a series of 25 bipolar scales (i.e., semantic differential scales). (From this, Yoshida calculated the absolute distance on each semantic scale.)

Results: Four dimensions were extracted, but not named:
1: Chanel No. 5 vs. White Rose (on opposite ends)
2: L'Origan vs. Arpège (on opposite ends)
3: Arpège vs. Cypre (on opposite ends)
4: Not specified

Yoshida–Experiment V (1964)

Odorants tested: Spices (including garlic, allspice, laurel, clove, paprika, cinnamon, thyme, sage, mace, fennel, cardamon, white pepper, ginger, black pepper, nutmeg)

Subjects: 5 males and 7 females

Results: Four dimensions were extracted:
1: Black pepper vs. fennel
2: Garlic vs. ginger
3: Ginger and white pepper vs. thyme and clove
General: one cluster of nuts and seeds and another cluster of garlic and ginger

Yoshida–Experiment VI (1964)

Odorants tested: Odors and malodors (including jasmin, scatol, heliotropin, vanillin, caproic acid, camphor, lemon bergamot, trimethyl amine, cassia, acetic acid, menthol, coffee, isovaleric acid, musk ambrette, carbol, amyl alcohol, terpene, indol, and anisaldehyde)

Subjects: 1 male and 4 females

Method: Direct judgment of similarity among all pairs

Results: Four dimensions were extracted:
1: Pleasant/unpleasant (terpene, camphor and menthol at the pleasant end vs nitrogeneous odorants, such as scatol, trimethylamine, indol at the other end)
2: Sweetness/pungent (sweet—vanillin, pungent—carbol, trimethylamine, carbol)
3 and 4: Evident, but not interpretable

Yoshida–Experiment VII (1964)

Odorants tested: Representative perfume chemicals, based upon Kainshow's classification scheme (scatol, olibanum, camphor, and citral)

Subjects: Two specialist perfumers, one male, one female, and another group of 6 naive panelists (1 male, 1 female)

Method: Direct judgment of similaritiy

Results: Three meaningful dimensions were extracted (although 6 factors in toto were statistically extracted):
1: Resinous burnt vs sweet
2: High pitched vivid odors vs heavy, base notes
3: Could not be interpreted

Yoshida–Experiment VIII (1964)

Odorants tested: Same as in VI and VII (in toto).

Subjects: 20 female subjects

Method: All stimuli on each of 25 bipolar scales

Results: Three dimensions were extracted:
1: Dynamism, sensory pleasure
2: Harshness
3: Vividness

(Note: In this study the odorants merely served as convenient stimuli. The real analysis was to find, from the set of 25 bipolar scales, how many base or primary scales there were. Yoshida found 3 such scales.)

Berglund, Berglund, Engen and Ekman (1972)

Odorants tested: 21 odorants, spanning a range of pleasant to unpleasant, high molecular weight, low molecular weight odors. All of the odorants were matched to have equal subjective intensity (40% as strong, subjectively, as the odor of undiluted acetone). Among the chemicals were acetone, amyl acetate, anethole, benzaldehyde, benzyl acetate, butanol, butyric acid, ethyl acetate, ethyl methyl ketone, eugenol, furfurole, geranial, guaiacol, heptane, heptanol, menthol, methyl salicylate, nonane, octane, 2 phenyethanol, iso-valeric acid.

Subjects: 11 subjects, who were somewhat sophisticated in sensory analysis of odors

Method: Direct similarity estimates on a 0-100 point scale, for all pairs

Results: They obtained large individual differences in the similarity judgments and concluded that we live in different olfactory worlds. The major factor that they isolated was hedonics, but the remaining individual factors were idiosyncratic to the individual.

Wright and Michels (1965)

Odorants tested: 50 odorants, spanning a wide range of types of odors and physical properties. The motive of the study originally was to test the hypothesis that there is a relation between odor quality and the Raman spectra of the odorant.

Subjects: 84 individuals

Method: Similarity of every one of the 50 test odorants to 9 standard odors (which varied in quality) using a 6 point scale

Results: 8 different axes or dimensions were found

1: Trigeminal (high—propionic acid, low—hydroxycitronellol)

2: Affective (low—pyridine, high—geraniol, undecanol)

3: Resinous (low—cyclopentane, thiophene; high—acetone, benzene, limonene)

4: Spicy (high—eugenol, low—pyridine, thiophene)

5: Benzothiazole (high—benzothiazole, skatole; low—eugenol)

6: Hexyl acetate (high—hexyl acetate, low—terpineol, turpentine)

7: Unpleasant poles (high—hydrogen sulfide)

8: Citral (high—citral, low—Lily of the Valley base)

Moskowitz and Gerbers (1974)

Odorants tested: 15 odorants, spanning a wide range of pleasant to unpleasant odorants, with different molecular properties. The odorants were previously matched to have approximately equal sensory intensity (acetophenone, benzaldehyde, butyl acetate, dl camphor, caproic acid, eugenol, guaiacol, isobutyl isobutyrate, isopropanol, limonene, methyl disulfide, methyl salicylate, pentanol, safrole, xylol)

Subjects: 15 individuals with moderate experience in sensory analysis

Method: Direct estimation of qualitative dissimilarity between all odors (15 x 14/2 = 105/ comparisons), qualitative dissimilarity between each odorant and 15 descriptor words (225 comparisons), and the qualitative dissimilarity between each odorant descriptor and every other descriptor (15 x 14/2 = 105). A total of 900 comparisons was obtained for each individual.

(In a second part of the study, the same individuals profiled each odorant on 17 descriptor terms, which comprised the same 15 terms they had used in dissimilarities estimation, along with two other terms.)

Results: A two dimensional space characterized both the dissimilarities ratings and the profile ratings. (The profile ratings were analyzed by unfolding methods.) Floral-animal and pleasant-unpleasant were the two major dimensions. In addition, the location of the odorants moved outwards in the odor space with increasing panelist experience. The authors concluded that odorants tend to become more qualitatively dissimilar to each other with repeated exposure, suggesting that the panelist picks out more points of difference between odors as the panelist experiences the odors.

Dravnieks (1974)

Odorants tested: 20 odorants, spanning a wide range of odor qualities. The odorants were selected to be equal in sensory intensity.

Subjects: 9 panelists were used. Each pair was judged twice by the panel of individuals.

Results: Dravnieks developed a model which considered the structural aspects of the molecule. That is, by looking at the geometrical space, one could ascertain what physical properties corresponded to the major dimensions which were recovered.

I: OH-heteroatoms, molecular size, positions and polarizability of polarizable bonds

II: Deals with multiple bonds, but does not need anything concerning the presence or absence of oxygen

III: Molecular size, concerns the effect of the sulfur atom, and promotes the significance of the ether oxygen

IV: Concerns shape, bond polarizability, and the presence of OH and halogen atoms

Schutz (1964)

Odorants tested: 30 qualitatively dissimilar chemicals were profiled on 29 different attributes

Examples of odorants: Methanol, 1-menthol, 2 propanol, P dichlorobenzene ethyl acetate, benzaldehyde, I-heptanol, iso-safrole, 1-pentanol, skatole, 1-hexanol, eugenol, vanillin, pyridine, diethyl sulfide, methyl salicylate, guaiacol, amyl acetate, butylamine, 1-butanol, butyric acid, methyl ethyl ketone, benzyl acetate, 2-picoline, coumarin, 1-propanol, 1-octanol, benzyl benzoate, geraniol, ethanol

Subjects: Twenty individuals, six women and fourteen men, with previous experience in odor evaluation. Some were chemists, others were not.

Scaling: Category scale

Results: Extracted nine dimensions

1: Fragrant (methyl salicylate, benzyl acetate, iso-safrole)

2: Etherish (1-propanol, methyl ethyl ketone, ethanol)

3: Sweet (methanol, 1-butanol, vanillin)

4: Burnt (guaiacol, eugenol, skatole)

5: Rancid (butyric acid, skatole, octanol)

6: Oily (heptanol, octanol, pentanol)

7: Metallic (hexanol, ethyl acetate, butanol)

8: Spicy (benzaldehyde, amyl acetate, pyridine)

9: Sulfurous (butyric acid, eugenol, ethyl sulfide)

(Note: Two dimensions (fragrant, burnt) were the same as the Crocker-Hendersen system.)

Engen (1964)

Odorants tested: Various combinations of heptanal (oily) and amyl acetate (banana smell) mixed in varying proportions

Subjects: 13 individuals (each of whom compared the similarity of the mixtures to amyl acetate), and 11 other individuals (each of whom compared the similarity of the mixtures to heptanol)

Results: A factor analysis of the matrix of similarity judgments was done. Two factors were found. One factor was proportional to the percent of amyl acetate in the mixture, and the other factor was proportional to the amount of heptanol in the mixture. In both factors, the relation between loading on the factor and percent concentration appeared to be an S shaped curve.

Woskow (1968)

Odorants tested: 25 odorants (methyl salicylate, eugenol, pyridine, safrole, benzaldehyde, guaiacol, citral, n-butanol, toluene, anisole, n-propanol, acetic acid, n-pentanol, skatole, ethanol, n-butyric acid, n-nonanol, phenylethanol, vanillin, l-menthol, d-camphor, n-hexanol, pinene, n-octanol, n-heptanol).

Subjects: 20 unpracticed individuals

Scaling: Instructed subjects to categorize the degree of similarity between all pairs (l-most dissimilar, 9-most alike). All subjects rated each pair.

Results: Three dimensions were extracted

1: Hedonics (liking/disliking) (pyridine vs vanillin)

2: Cool, woody (d-camphor vs n-octanol)

3: No interpretation given

Moskowitz and Barbe (1976)

Odorants tested: 20 food odors, each diluted to 1% of its starting concentration, and 20 names of foods (ideal odor concepts). The odorants were lemon oil, green bell pepper, molasses, pineapple, bacon, tomato, allspice, chocolate, raspberry, apple, ginger, parmesan cheese, celery, beef, cherry, strawberry, sausage, anise, almond, cantoloupe.

Subjects: 13 individuals with some previous experience.

Scaling: Magnitude estimation to evaluate overall disimilarity (0-identical)

Results: The M-D-SCAL 5M program (Kruskal and Carmone, 1969) found two dimensions. One was fruit vs beef, the other was food vs spice. In addition, for some aromas the concept (treated as an aroma) was located almost in the identical spot as the aroma (no dissimilarity at all; eg, lemon oil as an odorant, ideal lemon odor as a concept). For other aromas, the concept and the aroma were dissimilar to each other (sausage, raspberry). In addition, an individual differences analysis (INDSCAL, Carrol and Chang, 1969) showed that the individuals tended to perceive the dissimilarities identically. (This contrasts sharply to what Berglund found for individual differences in the estimates of chemical odor similarities and dissimilarities where there were striking and overwhelming interindividual differences.)

Moskowitz, Dubose, Dravnieks and Reuben (1976)

Odorants evaluated: 2 sets of four odorants each. In each set the odorants were evaluated in singles, pairs, triples, and one four-component mixture. For study I, the odorants were butyric acid, guaiacol, limonene and methyl salicylate. For study II, the odorants were methyl propionate, propyl propionate, pentyl propionate, and iso-pentyl propionate. In each study, there were 15 concepts evaluated as odors as well.

Subjects: 8 moderately practiced subjects

Method: Magnitude estimates to reflect degree of dissimilarity (0-qualitative indentity)

Results: Two dimensions emerged in each study. In study I, the dimensions were pleasant vs unpleasant, and sharp/disinfectant vs smoky, burnt and woody. In study II, the dimensions were fruity vs chemical, and pungent/sharp vs disinfectant/flowery/heavy. In addition, mixtures lay closer to the center of the geometrical space, and single odorants were placed more toward the outside.

Moskowitz (1976)

Odorants evaluated: 31 odorants, comprising all possible combinations of 5 odorants (methyl salicylate, caproic acid, isobutyl isobutyrate, methyl disulfide, camphor). Also evaluated a set of 11 concepts as ideal odors.

Subjects: 14 subjects participated. Each had had some previous experience in evaluating dissimilarities.

Scaling: Magnitude estimates to reflect the degree of dissimilarity (0-qualitative identity)

Results: Two dimensions emerged. I: hedonics (liking/disliking) II: chemicals vs food/spice

In addition, mixtures lay intermediate in the middle of the space, whereas pure odorants lay towards the outside. An analysis of individual differences via the INDSCAL program revealed modest interindividual differences. An analysis of the data across replicates revealed a high individual consistency from one replicate to another.

Moskowitz (1974)

Odorants evaluated: 8 odorants at each of three levels: methyl salicylate, benzaldehyde, anethole, ethyl cinnamate, eugenol, propanol, guaiacol, citral

Subjects: 12 scientists and engineers

Method: Subjects rated the overall dissimilarity of all pairs at a fixed intensity level, using a scale of 0 (identity) to 1.0 (maximal dissimilarity).

Results: Two clusters of odorants emerged. One cluster comprised the sweet, fragrant, flowery and typically pleasant odors; the other cluster could not be easily named.

Alabran, Moskowitz and Mabrouk (1975)

Odorants evaluated: 31 stimuli, 28 of which had been previously identified as constitutents in carrot-root oil. The other 3 odorants were a natural occurring oil, a synthetic mixture, and the word "carrot."

Subjects: 22 female and three male subjects

Method: The subjects profiled the odorants on a list of 52 attributes each, using a 7 point scale of percent appropriate (0, 20, 40, 60, 80 and 100%). The analysis used an unfolding procedure which placed odorants and descriptor terms in a joint space.

Results: Two primary dimensions emerged. Dimension I had as opposites spicy/minty odors and terms vs moldy, oil and unpleasant descriptors and odors. Dimension II had as opposites food vs chemical odors and descriptors.