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Some algebraic aspects of Analysis of Variance

1. Basic notions

a/ Factor, nesting, crossing

A protocol of n numerical observations will be formally defined as a mapping $x : I \to \mathbb{R}$, where $|I| = n$: x is a vector element of the n-dimensional vector space $\mathbb{R}^I$ (set of all real-valued mappings from I to $\mathbb{R}$). We shall call x the <u>vector of observations</u>.

Let $f_A : I \to A$ be a <u>description of I</u> : we shall say that A is a <u>factor</u> if f_A is onto, that is if $f_A(I) = A$. Let $n_a = |f^{-1}(a)|$: $(n_a)\, a \in A$ defines a positive measure on A which is the image (by f_A) of the counting measure on I. We call n_a the <u>frequency measure</u> associated with factor A. The mapping f_A, hence the frequency measure n_a, are determined by the design of the experiment. We see that A is a factor if and only if $\forall a \in A : n_a > 0$. Last, we have the relation: $\sum_A n_a = n$.

Using the formal definition of a factor we can give formal definitions of the following relationships between factors: nesting and crossing.

<u>Nesting</u> : given two factors A and B, A will be said to be <u>nested within B</u> if there is a mapping $h : A \to B$ such that $f_B = h \circ f_A$ (composed mapping)

$$\begin{tikzcd} & A \arrow[dr, dashed, "h"] & \\ I \arrow[ur, "f_A"] \arrow[rr, "f_B"'] & & B \end{tikzcd}$$

<u>Crossing</u> : given two factors A and B, A and B will be said to be <u>crossed</u> if the cartesian product $A \times B$ is itself a factor. In other words: consider the mapping $f_{AB} : I \to A \times B$ defined by $f_{AB}(i) = (f_A(i), f_B(i))$: A and B are crossed if the mapping f_{AB} is onto, that is if $f_{AB}(I) = A \times B$. Let $n_{ab} = |f_{AB}^{-1}(a, b)|$: then A and B are crossed if and only if $\forall (a, b) \in A \times B : n_{ab} > 0$.

b/ Measures and (real-valued) mappings on a factor A

Let A be a factor and let c be a (positive or negative or signed) measure on A : c is entirely determined by the family $(c_a)\, a \in A$, where c_a is the measure of the one-element set $\{a\}$.

Let $\mathbb{R}^A$ be the set of all (real-valued) mappings on A, and let $\mathbb{R}_A$ be the set of all measures on A : $\mathbb{R}_A$ can be identified with the dual vector space of the vector space $\mathbb{R}^A$: $\mathbb{R}_A = (\mathbb{R}^A)^*$. If c is a measure on A and y a (real-valued) mapping on A, we can thus define the scalar product $\langle c, y \rangle = \sum_a c_a\, y(a)$.

Then, there is a isomorphism $\varphi: \mathbb{R}_A \to \mathbb{R}^A$ which is canonically associated with the frequency measure n_a: this isomorphism φ transforms a measure c onto its density with respect to n_a, that is onto the mapping $y: A \to \mathbb{R}$ defined by $\forall a \in A: y(a) = \frac{c_a}{n_a}$. By means of this isomorphism, one can define a unique <u>scalar product</u> associated with n_a on each of the spaces $\mathbb{R}^A$ and $\mathbb{R}_A$:

- for two (real-valued) mappings y and z: $\langle y, z \rangle = \sum_A n_a\, y(a)\, z(a)$
- for two measures c and d: $\langle c, d \rangle = \sum_A \frac{c_a d_a}{n_a}$.

We shall say that a measure and a mapping, or two mappings, or two measures are <u>orthogonal</u> (with respect to the measure n_a) if one of the above scalar products is zero.

c/ <u>'Lifting' a mapping or a measure</u>

Let A be a factor nested in a factor B; the preceding definitions apply to each factor and B with the frequency measures n_a and n_b.

If $h: A \to B$, the subset of A: $h^{-1}(b)$ will be denoted $A(b)$ (Read: A within b, or A for b). Then $\forall b \in B: n_b = \sum_{a \in A(b)} n_a$.

Now let y_B be a (real-valued) mapping on B: $y_B: B \to \mathbb{R}$. Let us define a (real-valued) mapping on A: $y_A: A \to \mathbb{R}$ by the formula $y_A = y_B \circ h$ (composed mapping), that is, $\forall a \in A(b): y_A(a) = y_B(b)$: by constructing y_A from y_B we shall say that we have 'lifted' the mapping y_B from B to A:

$$\begin{tikzcd} A \arrow[d, "h"'] \arrow[dr, dashed, "y_A"] & \\ B \arrow[r, "y_B"'] & \mathbb{R} \end{tikzcd}$$

Using now the isomorphism between measures and mappings, we can define the 'lifting' of a measure on B onto a measure on A in the following way: Let c_b be a measure on B; its density is a mapping, whose value is $\frac{c_b}{n_b}$. By definition, the lifted measure of c_b will be a measure c_a on A, whose density with respect to n_a is the lifted mapping of $\frac{c_b}{n_b}$. Hence the density with respect to n_a of the lifted measure is $\forall a \in A(b): \frac{c_b}{n_b}$, and the lifted measure itself is defined by $\forall a \in A(b): c_a = n_a \frac{c_b}{n_b}$.

Notice that the canonical character of the procedure of lifting ensures that <u>the scalar product is preserved by lifting</u>. For instance, if y_B and z_B are mappings on B: $\langle y_B, z_B \rangle = \sum_B n_b\, y_B(b)\, z_B(b)$. Now if y_A and z_A are the lifted mappings: $\langle y_A, z_A \rangle = \sum_A n_a\, y_A(a)\, z_A(a) = \sum_B \sum_{A(b)} n_a\, y_B(b)\, z_B(b)$

$$= \sum_B y_B(b)\, z_B(b) \sum_{A(b)} n_a = \sum_B y_B(b)\, z_B(b)\, n_b = \langle y_B, z_B \rangle.$$

2.- Contrasts and comparisons.

a/ Definitions

Sometimes the terms of 'contrast' and 'comparison' are used as synonyms; here we shall give to these two terms quite distinct definitions. The basic definitions will be the following ones:

i) a contrast on a factor A is defined as a measure on A whose total mass is zero, that is: c_a is a contrast on A if and only if $\sum_A c_a = 0$

ii) The set of all contrasts on A is a vector subspace of $\mathbb{R}_A$: we shall call it the overall comparison on A.

iii) Any vector subspace of the overall comparison on A will be called a comparison on A.

We then give some subsidiary definitions and properties: the dimension of a comparison (dimension of a vector space) will be called the number of degrees of freedom (d.f.) of the comparison. It is easily verified that the overall comparison on A has $|A|-1$ d.f. A comparison having a number of d.f. less than $|A|-1$ will be called a partial comparison on A. A comparison with 1 d.f. will be called unidimensional.

If V and V_1 are comparisons, and if V_1 is a vector subspace of V, V_1 will be called a subcomparison of V. If V_1 is a subcomparison of V, we define the residual comparison of V_1 with respect to V as being the supplementary orthogonal vector subspace of V_1 with respect to V; this residual comparison will be denoted $V-V_1$. If V_1 and V_2 are two linearly independent comparisons, we define their direct sum, which will be denoted $V_1 \oplus V_2$. If V_1 and V_2 are orthogonal, their direct sum will be denoted as a ordinary sum: V_1+V_2. If $V=V_1+V_2$, we say that V_1 and V_2 constitute an orthogonal decomposition of V.

A comparison on A with p d.f. can be generated by a basis of p linearly independent contrasts $(c_a^j)_{j=1,2,\ldots p}$. If the contrasts c_a^j are orthogonal, the basis will provide an orthogonal decomposition of the comparison into p unidimensional comparisons: $V=\sum_{j=1}^{p} V_j$.

b/ Lifting contrasts and comparisons

Let A be a factor nested in a factor B. Let c_β be a contrast on B. We can lift this contrast (which is a measure on B) onto a measure c_a on A as described in §c. It is easily verified that the measure c_a is itself a contrast on A — Proof:

$$\sum_A c_a = \sum_A c_\beta \frac{n_a}{n_\beta} = \sum_B \sum_{A(B)} c_\beta \frac{n_a}{n_\beta} = \sum_B \frac{c_\beta}{n_\beta} \sum_{A(B)} n_a = \sum_B \frac{c_\beta}{n_\beta} n_\beta = 0.$$

Owing to this property we can speak of a 'contrast on B' as meaning indifferently either the contrast on B itself or the lifted contrast on A.

Let us now take a comparison on B: by lifting each contrast of this comparison, we construct a comparison on A which will be, by definition, the 'lifted comparison' on A. We then speak of a 'comparison on B' as meaning either the comparison on B itself or the lifted comparison on A.

c/ Sums of squares (S.S.)

Let V be a comparison, y be the orthogonal projection of the vector of observations on the subspace V: then by definition the square of the length of this projection, that is, $(\langle y, y \rangle)^2$ will be the sum of squares (S.S.) associated with comparison V.

If we have an orthogonal decomposition of V, the SS. associated with V is the sum of the SS associated with the components, that is: additivity of vector spaces implies additivity of SS.

If c_a is a contrast on A, it generates a unidimensional comparison on A; the SS associated with this unidimensional comparison is easily seen to be: $\dfrac{(\sum_A c_a m_a)^2}{\sum_A \frac{c_a^2}{n_a}}$, where m_a is the mean of the observations for the level a of factor A.

Hence, the following very straightforward method for computing the S.S. associated with a comparison on V (with p d.f.) on a factor A:

- Choose an orthogonal basis of p contrasts: (c_a^j) $j = 1, 2, \dots p$.
- Compute the sum of the p S.S. associated with the p unidimensional comparisons:

$$SS(V) = \sum_{j=1}^{p} \frac{(\sum_A c_a^j m_a)^2}{\sum_A \frac{c_a^{j\,2}}{n_a}}$$

We shall call this method of computing S.S. the method of contrasts.

3. Decomposition of a crossing

In what follows we use the same letters $A, B\ldots$ to denote factors and the overall comparisons on these factors.

Let A and B be two crossed factors. To the factor $A\times B$ we associate the frequency measure n_{ab}; to factor A we associate the frequency measure $n_a = \sum_B n_{aB}$ et to factor B the frequency measure $n_b = \sum_A n_{aB}$.

a/ Main effects

We can always define the main effects comparisons A and B, but in general these two comparisons will not be orthogonal. We have the following theorem:

Theorem: the comparisons A and B are orthogonal if and only if the design is orthogonal with respect to A and B, that is if the measure n_{aB} satisfies the condition $\forall (a,b)\in A\times B$: $n_{ab} = \frac{n_a n_b}{n}$

The proof of the 'if part' is straightforward: let c_a be a contrast on A and d_b be a contrast on B. Let us lift c_a onto $A\times B$; we get the contrast on $A\times B$ defined by $c_{ab} = n_{aB}\frac{c_a}{n_a}$. Similarly, if we lift d_b onto $A\times B$ we get the contrast $d_{ab} = n_{aB}\frac{d_b}{n_B}$.

Hence the scalar product of the two contrasts (with respect to the n_{aB} measure) is

$\langle c,d\rangle = \sum_A\sum_B \frac{c_{aB}d_{ab}}{n_{aB}} = \sum_A\sum_B \frac{c_a d_b}{n_a n_B} n_{aB}$. If $n_{aB} = \frac{n_a n_B}{n}$, $\langle c,d\rangle = \sum_A\sum_B \frac{c_a d_b}{n}$ $= \frac{1}{n}\sum_A c_a \sum_B d_b = 0$.

The proof of the 'only if' part follows from elementary classical results on measure spaces.

b) Interaction

Definition: the interaction comparison between A and B, denoted $A.B$, is defined as the residual comparison of the direct sum $A\oplus B$ with respect to $A\times B$ (that is, $A.B$ is the comparison on $A\times B$ orthogonal to both A and B); thus by definition

$$A.B = A\times B - (A\oplus B)$$

(Notice we use the symbol $\cdot$ for interaction as opposed to the symbol $\times$ for cartesian product)

If the design is orthogonal, A, B and $A.B$ constitute an orthogonal decomposition of $A\times B$, that is: $A\times B = A + B + A.B$

c) Basis of contrasts for the interaction comparison

Let c_a be a contrast on A, d_B be a contrast on B. Let $e_{aB} = c_a d_B$: it is easily proved that e_{aB} is an interaction contrast.

Now consider a basis of contrasts for comparison A and a basis of contrasts for comparison B. By multiplying term by term each contrast on A by each contrast on B we get a <u>basis for the interaction comparison.</u>

If the design is orthogonal and if one chooses an orthogonal basis on A and an orthogonal basis on B, it is easy to verify that this basis of the interaction is also orthogonal.

If the design is not orthogonal, the basis of interaction will not be orthogonal, but from this basis one will easily construct an orthogonal basis, using a suitable version of some well-known algorithm such as the Gram-Schmidt orthogonalization algorithm.

Using then the method of contrasts, we have a straightforward method for computing the SS of interaction; this method can be more convenient in many cases than the methods proposed by authors like Scheffé or Rao.

4. <u>A computer program</u> (simplified presentation)

<u>Rationale</u>: for a given type of design (say, some version of the randomized block design) the usual programs provide the standard decomposition (into orthogonal comparisons) which is directly determined by the structure of the design.

From the point of view of the data analyst, however: i/ these comparisons may not all be interesting — ii) other comparisons may be interesting. The standard decomposition is usually too gross for the experimentalist, who is often interested in partial comparisons on factors; guided by his hypotheses and by the aims of the experiment, he may, for instance, be interested in comparing two specified levels of a factor, or consider the linear trend on a given factor, or wish to test a factor within the different levels of another factor: all these comparisons usually do not fit <u>together</u> in the same standard decomposition.

Hence the idea of <u>more versatile programs</u>, which would concentrate on the comparisons of interest for the experimentalist.

We have thus written a computer program which tends to respond to these needs and uses the properties of contrasts and comparisons described earlier in this paper.

This program relates to the randomized block design, in which a random factor S ('subjects') is nested within a fixed factor G ('groups' or blocks) and crossed with another fixed factor T ('treatments') (For a typical version of the program, $|G| = 10$, $|T| = 100$.) Naturally, G and T are themselves (usually) combinations of more primitive factors (for instance, T can be the cartesian product of two crossed factors: $T = A \times B$, etc.)

In this program, it is assumed that the user is interested in a certain number of prespecified comparisons on the cartesian product $G \times T$ which can be described by means of comparisons on G and/or comparisons on T.

For each prespecified comparison, the user provides an orthogonal basis of contrasts on G and/or an orthogonal basis of contrasts on T.(*) The computer 'lifts' each comparison on $G \times T$ and computes the associated S.S. by the method of contrasts. It also computes various denominators ('error terms') specifically associated with the comparison, and proposes the different F ratios corresponding to these denominators. The user of the program can then choose ~~among~~ these F ratios by taking into account statistical properties such as validity and power.(**)

(*) To instruct such bases he can use a preliminary program which generates contrast bases for the most commonly made comparisons (main effects, interactions, components of regression, etc).

(**) Cf Rouanet and Lépine: 'Comparisons between treatments in a repeated-measurement design', British J. of Math. and Stat. Psychol., 23, 1970, 147-163