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Abstract
We consider designs with t treatments, the ith of which has n_i observations. Four cases are examined: treatments both ordered and not, and the design balanced, with all n_i equal, and not. A general construction is given that takes observations, typically treatment sums or treatment rank sums, constructs a simple quadratic form and expresses it as a sum of squares of orthogonal contrasts. For the case of ordered treatments, the Kruskal-Wallis, Friedman and Durbin tests are recovered by this construction. A data set where the design is the supplemented balanced, which is an unbalanced design, is analyzed. When treatments are not ordered the construction also applies. We then focus on Helmert contrasts.

KEYWORDS*:* balanced incomplete block designs; completely randomised design; Helmert matrices; Latin square design; supplemented balanced design; randomised block design

AMS SUBJECT CLASSIFICATION CODES: 62G; 62F

1. Introduction

Thas et al. (2012) showed how to construct orthogonal contrasts for the completely randomised, randomised block and balanced incomplete block designs by decomposing, respectively, the Kruskal-Wallis, Friedman, and Durbin test statistics into sums of squares of orthogonal contrasts. However their approach only works for balanced designs in which each of the ordered treatments is observed the same number of times. The construction given subsequently gives orthogonal contrasts for both ordered and unordered treatments and both balanced and unbalanced designs. The sum of squares of these contrasts is a simple quadratic form that may be used as an omnibus test statistic, or, for example, to calculate a residual. The construction may be such that the quadratic form is a rank test statistic or a treatment sum of squares in an ANOVA.

The construction is described in sections 2 and 3. It takes the treatment (rank) sums, standardizes and normalizes them, generates orthogonal contrasts and aggregates them into a simple closed form. Asymptotically the aggregated statistic has the χ^2 distribution and the contrasts are orthogonal, each with the χ_1^2 distribution. Unordered treatments are considered in section 4. Familiarity with the material in Thas et al. (2012) will assist the reader.

To end this introduction we give an example to demonstrate the decompositions given here. The RL statistic used in this example was proposed in Livingston and Rayner (2022) and Rayner and Livingston (2022). It is a rank sum statistic to analyze Latin square data and, as will be shown, is consistent with the construction described in the next section. Since the Latin square design is balanced the orthogonal contrasts could also have been derived using the approach in Thas et al. (2012). The recommended test first aligns and then ranks the raw data.

Traffic Example. Kuehl (2000, p.301) considers the scenario in which a traffic engineer conducts a study to compare the total unused red-light time for five different traffic light signal sequences. The experiment was conducted with a Latin square design in which blocking factors were (1) five intersections and (2) five time of day periods. In Table 1 the five signal sequence treatments are shown in parentheses as A, B, C, D, E and the numerical values are the unused red-light times in minutes.

Table 1. Unused red-light time in minutes.

	Time Period				
Intersection	1	2	3	4	5
1	15.2 (A)	33.8 (B)	13.5 (C)	27.4 (D)	29.1 (E)
2	16.5 (B)	26.5 (C)	19.2 (D)	25.8 (E)	22.7 (A)
3	12.1 (C)	31.4 (D)	17.0 (E)	31.5 (A)	30.2 (B)
4	10.7 (D)	34.2 (E)	19.5 (A)	27.2 (B)	21.6 (C)
5	14.6 (E)	31.7 (A)	16.7 (B)	26.3 (C)	23.8 (D)

Rayner and Best (2011) report different analyses, both parametric and nonparametric, with treatment p-values both above and below 0.05. They also suggest the value 19.2 at intersection 2 and time period 3 might be an outlier.

A parametric analysis of the raw data gives a p-value of 0.0498 for treatments. The residuals are consistent with normality. Nevertheless the possible outlier suggests it may be informative to consider the ranks.

The ANOVA F test on the ranks gives a p-value of 0.0328 for treatments and a corresponding permutation test p-value of 0.0167. For the Latin square design we find χ^2 p-values unreliable and hence use permutation test p-values, here based on 1,000,000 permutations.

The aligned rank sums are 76, 94, 22, 54 and 79 for A to E respectively. Plots of these sums against treatments, ordered A to E, show a shape that is possibly cubic. Incidentally, the rank sums for the non-aligned data are 72, 74, 47, 62 and 70; alignment has made quite a difference, especially with the second and third sums.

The p-values of the RL test and its first, second, third, and fourth degree orthonormal contrasts were 0.0780, 0.5971, 0.1172, 0.1948 and 0.0680 respectively. The RL test is not significant at the 0.05 level. The detailed analysis here shows that at the 0.05 level only the degree four effect is approaching significance, and that is unlikely to be of interest to the traffic engineer.

To calculate the contrasts here and subsequently requires the calculation of orthonormal polynomials of multiple degrees. We use Emerson recurrence; see Emerson (1968) and Rayner et al. (2008).

2. The construction

In the following no constraints on the design are imposed, except that the definitions are meaningful. There may be several factors present, but we will focus on one that will be called treatments. Initially the treatments levels are assumed to be ordered. There are t treatment levels, with n_i observations of the ith, and n observations in all. The construction is developed for ranked data; modifications for unranked ordered data are immediate. The expression developed for G_O below is appropriate when ranking is overall. A slightly modified version, G_{WB}, is subsequently developed for when there is a single blocking factor and ranking is within blocks.

The raw (unranked) data are represented as y_{ij}, $j = 1, \ldots, n_i$ and $i = 1, \ldots, t$, the jth observation on the ith treatment. Initially we take r_{ij} to be the *overall* rank of y_{ij}. Suppose the sum of the ranks for treatment i is $R_i = \sum_{j=1}^{n_i} r_{ij}$, $i = 1, \ldots, t$, and that the sum of all the ranks is $T = \sum_{i=1}^{t} R_i$. If ties occur mid-ranks will normally be used. Provided the rank sum is preserved at $n(n + 1)/2$ – what it would have been with untied data – other ranking options may be used.

We now define a contrast. Suppose $c = (c_1, \ldots, c_t)^T$ is a vector of contrast coefficients and that $w = (w_1, \ldots, w_t)^T$ is a vector of variables or parameters. Then for balanced designs Thas et al. (2012) say $c^T w$ is a contrast if $c_1 + \ldots + c_t = 0$. However more generally we need to account for treatments with unequal numbers of observations. For $i = 1, \ldots, t$ put $p_i = n_i/n$ and redefine the contrast coefficients as $c = (p_1 c_1, \ldots, p_t c_t)^T$. Then $c^T w$ is a contrast if $p_1 c_1 + \ldots + p_t c_t = 0$. As an example suppose we have t samples with means $\bar{x}_1, \ldots, \bar{x}_t$. If n_i is the size of the ith sample then provided $n_1 c_1 + \ldots + n_t c_t = 0$ a contrast in the sample means is $p_1 c_1 \bar{x}_1 + \ldots + p_t c_t \bar{x}_t = (c_1 \sum_j x_{1j} + \cdots + c_t \sum_j x_{tj})/n$. For example, take $c_1 = n_2$ and $c_2 = -n_1$ so that a contrast involving the first two sample means is $(n_2 \sum_j x_{1j} - n_1 \sum_j x_{2j})/n = n_1 n_2 (\bar{x}_1 - \bar{x}_2)/n$. Note that if $c^T w$ is a contrast and f a constant, then $f c^T w$ is also a contrast.

With these definitions put $var = \sum_{i,j} r_{ij}^2 / n - \{(n + 1)/2\}^2$, the variance of the possibly tied ranks. Now for $i = 1, \ldots, t$ define the centred and normalised rank sums,

$$Z_i = (R_i - E[R_i])/\sqrt{n\ var}$$

in which E[R_i] = Tn_i/n, the proportion of the rank sum attributable to the ith treatment. Note that $\sum_i Z_i = 0$.

Write $Z = (Z_1, \ldots, Z_t)^{\mathrm{T}}$. Suppose that $p = (p_1, \ldots, p_t)^{\mathrm{T}}$ and that the p_i are positive and sum to one: $p_i > 0$ for $i = 1, \ldots, t$ and $\sum_i p_i = 1$. Now $\{h_r\}$, in which $h_r = (h_{r1}, \ldots, h_{rt})^{\mathrm{T}}$, $r = 1, \ldots, t$, is a set of orthogonal functions with weight function p provided E[$h_r\, h_s$] = δ_{rs}, that is, 1 for $r = s$ and zero otherwise, where the expectation is with respect to the distribution with probability function p. Explicitly, $\sum_j h_{rj} p_j h_{sj} = \delta_{rs}$.

As is customary we take the orthogonal function of degree zero to be identically 1, although we designate the tth function to be the degree zero orthonormal function to simplify subsequent notation: that is $h_t = 1_t$. It follows that $h_t^{\mathrm{T}} Z = 1_t^{\mathrm{T}} Z = \sum_i Z_i = 0$. The orthogonality of the $\{h_r\}$ means that for $r = 1, \ldots, t - 1$, $\mathrm{E}[h_r^{\mathrm{T}} h_t] = \delta_{rt} = 0 = \mathrm{E}[h_r] = \sum_i h_{ri} p_i$ so that the $h_r^{\mathrm{T}} Z = \sum_i h_{ri} p_i Z_i$ are contrasts. Since $\{h_r\}$ is orthonormal $\{h_r^{\mathrm{T}} Z\}$ are said to be orthonormal contrasts. As before, if for $r = 1, \ldots, t - 1$ the $h_r^{\mathrm{T}} Z$ are orthonormal contrasts and f is a constant, then the $f\ h_r^{\mathrm{T}} Z$ are also orthonormal contrasts.

Note that, as is common in the literature, we frequently say 'orthogonal contrasts' when the contrasts are, in fact, orthonormal. To proceed a lemma is needed. We previously defined $p_i = n_i/n$, a particular case of the q_i subsequently.

Lemma. Suppose that $h_1, \ldots, h_{t-1}$, $h_t = 1_t$ are $t \times 1$ vectors orthonormal with weight function $q = (q_1, \ldots, q_t)^{\mathrm{T}}$ in which all $q_i > 0$ and $\sum_i q_i = 1$. Define D = diag($q_1, \ldots, q_t$). Then

$$h_1 h_1^{\mathrm{T}} + \ldots + h_{t-1} h_{t-1}^{\mathrm{T}} = \mathrm{D}^{-1} - 1_t 1_t^{\mathrm{T}}.$$

Proof. Define H by $\mathrm{H}^{\mathrm{T}} = (h_1 | \ldots | h_{t-1})$ and H* by $\mathrm{H}^{*\mathrm{T}} = (\mathrm{H}^{\mathrm{T}} | 1_t)$. Then $\mathrm{H}^{\mathrm{T}}\mathrm{H} = h_1 h_1^{\mathrm{T}} + \ldots + h_{t-1} h_{t-1}^{\mathrm{T}}$. The orthonormality means that for $r, s = 1, \ldots, t$, $h_r^{\mathrm{T}} \mathrm{D} h_s = \delta_{rs}$, and hence that $\mathrm{H}^*\mathrm{D}\mathrm{H}^{*\mathrm{T}} = \mathrm{I}_t$. Put $\mathrm{K} = \mathrm{H}^*\mathrm{D}^{0.5}$. Then $\mathrm{K}\mathrm{K}^{\mathrm{T}} = \mathrm{I}_t$, so that K is an orthogonal matrix. Hence $\mathrm{K}^{\mathrm{T}}\mathrm{K} = \mathrm{I}_t = \mathrm{D}^{0.5}\, \mathrm{H}^{*\mathrm{T}}\, \mathrm{H}^*\, \mathrm{D}^{0.5}$ and $\mathrm{D}^{-1} = \mathrm{H}^{*\mathrm{T}}\, \mathrm{H}^*$. Thus $\mathrm{D}^{-1} = \mathrm{H}^{\mathrm{T}}\, \mathrm{H} + 1_t 1_t^{\mathrm{T}}$ and the stated result follows.

Now from the lemma, if Y is any $t \times 1$ vector with elements Y_i, then

$$(h_1^{\mathrm{T}} Y)^2 + \cdots + (h_{t-1}^{\mathrm{T}} Y)^2 = Y^{\mathrm{T}}(\mathrm{D}^{-1} - 1_t 1_t^{\mathrm{T}})Y = \sum_i \frac{Y_i^2}{q_i} - \left(\sum_i Y_i\right)^2.$$

This result requires no model.

We now apply the lemma to $\{Z_i\}$ and $\{p_i\}$ defined previously. Since $\sum_i Z_i = 0$ this gives a decomposition of $\sum_i Z_i^2/p_i = G_{\mathrm{O}}$ say, into squared components $(h_r^{\mathrm{T}} Z)^2$, $r = 1, \ldots, t - 1$:

$$G_{\mathrm{O}} = \sum_i Z_i^2/p_i = \sum_i (R_i - Tn_i/n)^2/(n_i\ var) = (h_1^{\mathrm{T}} Z)^2 + \cdots + (h_{t-1}^{\mathrm{T}} Z)^2.$$

The subscript 'O' is to indicate ranking is overall rather than within blocks.

The development for balanced designs in Thas et al. (2012) required, for their Y, $1_t^{\mathrm{T}}Y = 0$ to construct their contrasts. They then use the singular value decomposition theorem to show that their test statistics are the sum of squares of $t - 1$ contrasts. We can achieve the same result by putting $p_i = 1/t$ in the lemma.

We now turn to ranking within blocks. First note that if, as in the Latin square design, there is more than one blocking factor, then ranking within blocks is ambiguous. Hence the following assumes there is only one blocking factor as, for example, in the randomised block design. When ranking is overall the construction decomposes $\sum_i (R_i - Tn_i/n)^2/(n_i\ var)$ in which E[R_i] = Tn_i/n and $var = \sum_{i,j} r_{ij}^2/n - \{(n+1)/2\}^2$, the variance of the possibly tied ranks. When ranking is within blocks then we now define r_{ij} as the rank sum for treatment i in block j, so that $R_i = \sum_j r_{ij}$, the rank sum over blocks for treatment i. For E[R_i] instead of the proportion of the *overall* rank sum attributable to the ith treatment we need to aggregate the proportions of the *block* rank sums attributable to the ith treatment, $p_i \sum_j r_{ij}$. The aggregation is E[R_i] = $\sum_i p_i \sum_j r_{ij}$. Suppose there are b blocks in all, with b_j observations in block j. The construction is applied to $Z_i = (R_i - E[R_i])/\sqrt{\sum_j S_j}$ in which

$$b_j S_j = \sum_i r_{ij}^2 - \left(\sum_i r_{ij}\right)^2 / b_j$$

and gives

$$\left\{\sum_i (R_i - \mathrm{E}[R_i])^2/n_i\right\} / \sum_j S_j = (h_1^{\mathrm{T}}Z)^2 + \cdots + (h_{t-1}^{\mathrm{T}}Z)^2 = G_{WB} \text{ say.}$$

One advantage of defining G_{O} and G_{WB} as we have is that by so doing we recover tests such as the Kruskal-Wallis and Friedman. This is shown in the appendix.

3. Distribution theory

We now show that $Z^{\mathrm{T}}(\mathrm{D}^{-1} - 1_t 1_t^{\mathrm{T}})Z = G$ say, asymptotically has the χ_{t-1}^2 distribution and the contrasts are asymptotically uncorrelated. This follows when either ranking method, overall or within blocks, is used. Hence the notation, dropping the subscripts on G_{O} and G_{WB}.

As before we have D = diag(p_i). Put $W = (W_i) = \mathrm{D}^{-0.5}Z$, $u = D^{0.5}1_t$ and $\mathrm{A} = \mathrm{I}_t - uu^{\mathrm{T}}$. Then $G = W^{\mathrm{T}}AW$. Now $u^{\mathrm{T}}u = 1_t^{\mathrm{T}}D1_t = \sum_i p_i = 1$. Thus $\mathrm{A}^2 = \mathrm{I}_t - uu^{\mathrm{T}} - uu^{\mathrm{T}} uu^{\mathrm{T}}uu^{\mathrm{T}} = \mathrm{I}_t - uu^{\mathrm{T}} = \mathrm{A}$: A is idempotent. By the Central Limit Theorem the W_i are asymptotically N(0, 1). The eigenvalues of A are one $t - 1$ times and zero once. It follows that the rank of A is $t - 1$ and the distribution G is χ_{t-1}^2. As in Thas et al. (2012, Appendix A) the covariance matrix of Z is $\Sigma = h_1 h_1^{\mathrm{T}} + \cdots + h_{t-1}h_{t-1}^{\mathrm{T}}$ and $\mathrm{cov}(h_r^{\mathrm{T}}Z,\ h_s^{\mathrm{T}}Z) = h_r^{\mathrm{T}}\Sigma h_s = \delta_{rs}$: the $h_r^{\mathrm{T}}Z$ are uncorrelated. As a corollary the $(h_r^{\mathrm{T}}Z)^2$ are asymptotically χ_1^2 distributed.

In Thas et al. (2012) the objective was to decompose statistics known, at least asymptotically, to have the χ^2 distribution. Here that is not necessarily the case. As in the supplemented balanced example following it is the procedure that gives the omnibus test statistic $\sum_i Z_i^2$ and the construction that gives its distribution. In practice the χ^2 approximation to this sampling distribution may be poor. See the discussions for the Durbin and RL statistics in Rayner and Livingston (2022). In fact it may also be the case that while $\sum_i Z_i^2$ is well-approximated by the χ^2_{t-1} distribution, the squared contrasts $(h_r^{\mathrm{T}} Z)^2$ are not well-approximated by the χ^2_1 distribution.

The nett outcome of this discussion is that the χ^2 sampling distributions may not be available. From one perspective that is not too great a handicap: in such situations we can calculate p-values using resampling methods such as permutation testing. However if the χ^2_{t-1} distribution is dubious then so is the orthogonality of the contrasts and that means that effects of different significant squared contrasts are not independent. Thus a significant linear effect may induce a significant quadratic effect. Again this is not often a problem. Often the contrasts are being calculated more as exploratory data analytic tools, and formal conclusions from their use will augment subjective conclusions from tools such as data plots. See the strawberry example following.

Strawberry Example. Pearce (1960) considered the supplemented balanced design and gave an example using the strawberry data set in Table 2, in which there are five treatments and four blocks. The control occurs twice on each block while the other treatments occur twice on one block and once on the other blocks. Thus there are eight observations of the control and five of each of the other treatments. The experiment is unbalanced in our sense, but since there are seven observations on each block there is also a sense of balance that justifies Pearce's use of the term. The data can be ranked overall after first aligning to remove the block effects, or ranked within blocks. We do both. We also give permutation test p-values.

Pesticides are applied to strawberry plants to inhibit the growth of weeds. The response represents the total spread in inches of twelve plants per plot approximately two months after the application of the weedkillers. The question is, do they also inhibit the growth of the strawberries? There is an assumed treatment order: A → B → C → D → O.

Table 2. Growth of strawberry plants after applying pesticides.

Block I	Block II	Block III	Block IV
C, 107 (5)	A, 136 (14)	B, 118 (8)	O, 173 (23)
A, 166 (21.5)	O, 146 (16)	A, 117 (7)	C, 95 (1)
D, 133 (13)	C, 104 (4)	O, 176 (24)	C, 109 (6)
B, 166 (21.5)	B, 152 (18)	D, 132 (12)	A, 130 (10)
O, 177 (25)	D, 119 (9)	B, 139 (15)	D, 103 (2.5)
A, 163 (19)	O, 164 (20)	O, 186 (27)	O, 185 (26)
O, 190 (28)	D, 132 (11.5)	C, 103 (2.5)	B, 147 (17)

Each cell gives the pesticide, the response and the corresponding overall mid-rank.

Analysis in Rayner and Livingston (2022, Chapters 8 and 10) suggest a relationship between the means of the raw data that is predominantly quadratic with an element of linearity.

If the data are aligned before ranking overall then using the chi-squared distributions with permutation test p-values based on 10,000,000 permutations in parentheses, we find that the omnibus statistic has p-value 0.0001 (0.0000) while the p-values for the four orthogonal contrasts are 0.0433 (0.0416), 0.0005 (0.0002), 0.0278 (0.0254) and 0.1352 (0.1376) respectively. The aggregated effect is highly significant; the most dominant of the effects is the quadratic.

If instead the data are ranked within blocks the analysis yields very similar results. The chi-squared distribution p-values with permutation test p-values based on 10,000,000 permutations in parentheses finds the omnibus statistic has p-value 0.0002 (0.0000) while the p-values for the four orthogonal contrasts are 0.0401 (0.0501), 0.0017 (0.0017), 0.0128 (0.0149) and 0.1497 (0.1721) respectively. While the quadratic contrast is strong, so is the cubic, suggesting a complex relationship between the mean ranks.

For both methods of blocking the chi-squared p-values are generally similar to those based on the permutation distribution.

4. Orthogonal Contrasts for Unordered Means

Although we could give a more general exposition, suppose we have a one factor ANOVA with observations X_{ij}, $j = 1, \ldots, n_i$, $j = 1, \ldots, t$. Write $T_i = \sum_j X_{ij}$ and $T = \sum_{i,j} X_{ij}$. The factor, total and error sums of squares are given by $SSF = \sum_i T_i^2/n_i - T^2/n$, $SST = \sum_{i,j} X_{ij}^2 - T^2/n$ and $SSE = SST - SSF$ respectively.

Put $Z_i = T_i - Tn_i/n = n_i(\bar{X}_i - T/n)$ and as previously $p_i = n_i/n$, both for $i = 1, \ldots, t$. Then $\sum_i Z_i = 0$ and $\sum_i Z_i^2/p_i = nSSF$. If $\{h_r\}$ are orthonormal functions with weight function $\{p_i\}$ and if $h_1 = 1_t$, then as before, the $h_r^{\mathrm{T}} Z$, $r = 2, \ldots, t$, are contrasts. The procedure from section 2 gives $\sum_i Z_i^2/p_i = (h_2^{\mathrm{T}} Z)^2 + \cdots + (h_t^{\mathrm{T}} Z)^2$, and we also have that this is $nSSF$.

A useful approach is to construct orthonormal functions from orthogonal matrices. Suppose $p_i > 0$ for $i = 1, \ldots, t$ and $\sum_i p_i = 1$. Put $\mathrm{D} = \mathrm{diag}(p_1, \ldots, p_t)$ and suppose V is an orthogonal matrix with first row $(\sqrt{p_1}, \ldots, \sqrt{p_t})$. Define $\mathrm{H} = \mathrm{V}\,\mathrm{D}^{-0.5}$ and suppose $\mathrm{V}^{\mathrm{T}} = (v_1| \ldots|v_t)$ and $\mathrm{H}^{\mathrm{T}} = (h_1| \ldots|h_t)$. The orthogonality of V gives $\mathrm{I}_t = \mathrm{V}\,\mathrm{V}^{\mathrm{T}} = \mathrm{H}\,\mathrm{D}\,\mathrm{H}^{\mathrm{T}}$ so that $h_r^{\mathrm{T}} \mathrm{D} h_s = \delta_{rs}$: the $\{h_r\}$ is orthonormal with weight function $(p_1, \ldots, p_t)^{\mathrm{T}}$. Moreover the first row of H, h_1^{T}, is $h_1^{\mathrm{T}} \mathrm{D}^{-0.5} = 1_t^{\mathrm{T}}$. The construction of section 2 now applies with the $\{h_r^{\mathrm{T}} Z\}$ the orthonormal contrasts.

One option in statistical analysis is to use the Helmert matrices (Lancaster, 1965) to construct Helmert contrasts. For positive p_i write $P_k = p_1 + \ldots + p_k$, $k = 1, \ldots, t$ so that $P_t = 1$. Then the Helmert matrix V is given by

$$v_{1j} = \sqrt{p_j},\ v_{ij} = 0 \text{ for } j > i > 1,$$
$$v_{ii} = -\sqrt{P_{i-1}/P_i} \text{ and } v_{ij} = \sqrt{p_i p_j/(P_i P_{i-1})} \text{ for } i > j,\ i > 1.$$

As above put $\mathrm{H} = \mathrm{V}\,\mathrm{D}^{-0.5}$. Then $h_{1j} = 1$ for $j = 1, \ldots, t$. For $r = 2, \ldots, t$ the h_r are orthonormal functions that lead to contrasts that compare the first r Z_i. We have

$$h_{r1} = \sqrt{p_1/(P_r P_{r-1})},\ h_{r2} = \sqrt{p_2/(P_r P_{r-1})},\ \ldots,\ h_{r,r-1} = \sqrt{p_{r-1}/(P_r P_{r-1})},$$

$$h_{r,r} = -\sqrt{P_{r-1}/(p_r P_r)} \text{ with } m_{r,j} = 0 \text{ for } j > r > 1.$$

Thus for $r = 2, \ldots, t$ the rth Helmert contrast, $h_r^{\mathrm{T}} Z$, is given by

$$h_r^{\mathrm{T}} Z = Z_1\sqrt{p_1/(P_r P_{r-1})} + \cdots + Z_{r-1}\sqrt{p_r/(P_r P_{r-1})} - Z_r\sqrt{P_{r-1}/(p_r P_r)}.$$

In the one factor ANOVA since $SSF = \{(h_1^{\mathrm{T}} Z)^2 + \cdots + (h_{t-1}^{\mathrm{T}} Z)^2\}/n$, the contrasts decompose the treatment sum of squares. The rth contrast test statistic, $r = 2, \ldots, t$, is $(h_r^{\mathrm{T}} Z)^2/(nSSE)$ and has the $F_{1,n-t}$ distribution.

For many data sets the Helmert contrasts may not be relevant. The usual process is the context determines which contrasts of interest, and this leads to a set of linearly independent vectors to which the Gram-Schmidt orthogonalisation process can be applied to construct the orthonormal vectors, starting with $(\sqrt{p_1}, \ldots, \sqrt{p_t})^{\mathrm{T}}$.

The Ordered Effect of Alcohol on Anxiety Example. Five groups of 50 year-old adults were administered between 0 and 4 ounces of pure alcohol per day over a one-month period. At the end of the experiment, their anxiety scores were measured with a well-known anxiety scale. At the time of writing the data were available at 5-63 from https://www.marekrychlik.com/sites/default/files/05_contrasts1.pdf

Table 3. Anxiety scores for different alcohol consumptions.

Alcohol	Anxiety score						
0oz	115	133	110	125			
1oz	99	92	103	105	120		
2oz	91	103	109	98	100	93	106
3oz	84	83	87	95	64		
4oz	99	93	87	88	112		

An ordered analysis gives the χ^2 p-values (with permutation test p-values in parentheses) for the contrasts of degree one, two, three and four and the omnibus statistic were 0.0015 (0.0000), 0.0749 (0.1901), 0.3963 (0.3200), 0.1609 (0.2398) and overall 0.0032 (0.0004) respectively. The mean anxiety scores for the different alcohol levels are 120.75, 103.8, 100.0, 82.6 and 95.8. There is a strong linear (downward) effect with an upturn for the final treatment inducing a weak quadratic effect. The significant overall effect is barely diluted by the non-linear effects.

When the ordering of the treatments is ignored the Helmert contrasts χ^2 p-values (with permutation test p-values in parentheses) were 0.0015 (0.0154), 0.0749 (0.0284), 0.3962 (0.0005), 0.1609 (0.3132) and overall 0.0032 (0.0007). The first Helmert contrast compares the first two treatments, the second compares the first two treatments with the third, and so on. Overall there is a significant difference in means, with the second, third and fourth means significantly different from their predecessors. Only the mean of the fifth treatment is not different from the mean of its predecessors.

Here the agreement between the χ^2 and permutation test p-values is not as good as for the supplementary balanced design. That being the case, more emphasis should be given to the permutation test p-values. Of course how good the agreement between χ^2 and permutation test p-values will depend on several factors, such as the sample size, the design and as the last two examples here suggest also, how unbalanced the design is.

References

Best, D.J. and Rayner, J.C.W. (2011). Nonparametric tests for Latin squares. NIASRA Statistics Working Paper Series, Paper 11-11.

Emerson, P.L. (1968). Numerical construction of orthogonal polynomials from a general recurrence formula. *Biometrics* 24, 695–701.

Kuehl, R. (2000). *Design of Experiments: Statistical Principals of Research Design and Analysis*. Belmont, California: Duxbury Press.

Livingston Jr, G. C. and Rayner, J.C.W. (2022). A rank test for the Latin square design. Submitted.

Pearce, S.C. (1960). Supplemented balanced. *Biometrika*, 47, 263-271.

Rayner, J.C.W. and Best, D.J. (2001). *A Contingency Table Approach to Nonparametric Testing*. Boca Raton: Chapman & Hall/CRC.

Rayner, J.C.W. and Livingston Jr, G. C. (2022). *An Introduction to Cochran–Mantel–Haenszel Testing and Nonparametric ANOVA*. Wiley. To appear.

Rayner, J.C.W., Thas, O. and De Boeck, B. (2008). A generalised Emerson recurrence relation. *Australian and NZ Journal of Statistics*, 50 (3), 235-240.

Thas, O., Best, D.J. and Rayner, J.C.W. (2012). Using orthogonal trend contrasts for testing ranked data with ordered alternatives. *Statisticia Neerlandica*, 66(4), 452-471.

Appendix. The method recovers important rank tests and their orthogonal contrasts

As above, if ranking is overall the construction is based, for i = 1, …, t, on $Z_i = (R_i - E[R_i])/\sqrt{n\ var}$, in which $var = \sum_{i,j} r_{ij}^2 /n - \{(n+1)/2\}^2$, the variance of the possibly tied ranks. If ranking is within blocks the construction is based on $Z_i = (R_i - E[R_i])/\sqrt{\sum_j S_j}$. We now show that specific cases of the construction yields the Kruskal-Wallis test statistic even when the design is not balanced, and the Friedman, Durbin and RL test statistics.

Completely Randomised Design

The Kruskal-Wallis test statistic is

$$KW_A = \frac{(n-1)\{\sum_i \frac{R_i^2}{n_i} - \frac{n(n+1)^2}{4}\}}{\sum_{i,j} r_{ij}^2 - \frac{n(n+1)^2}{4}}.$$

Since ranking is overall, preserving the rank sum however ties occur, $\sum_{i,j} r_{ij}$ = 1 + … + n = $n(n + 1)/2 = T$. Thus E[R_i] = (n_i/n) $n(n + 1)/2 = n_i(n + 1)/2$ and

$$\sum_i (R_i - Tn_i/n)^2/n_i \ = (\sum_i \frac{R_i^2}{n_i}) - T^2/n.$$

In the construction, as $var = \sum_{i,j} r_{ij}^2 /n - \{(n+1)/2\}^2$,

$$G_{\text{O}} = \frac{\sum_i (R_i - Tn_i/n)^2/n_i}{\sum_{i,j} r_{ij}^2 /n - \{(n+1)/2\}^2} = \frac{n}{(n-1)} KW_A = (h_1^{\text{T}}Z)^2 + \cdots + (h_{t-1}^{\text{T}}Z)^2.$$

As previously mentioned, multiplying orthonormal contrasts by the same constant results in another set of orthonormal contrasts. Since $h_u^{\text{T}}Z$, u = 1, …, t – 1 are orthonormal contrasts whose sum of squares is G_{O}, $h_u^{\text{T}}Z\sqrt{\frac{n-1}{n}}$, u = 1, …, t – 1 are orthonormal contrasts whose sum of squares is KW_{A}.

Balanced Incomplete Block Design

The adjusted Durbin statistic is given by

$$D_A = \frac{(t-1)\{\sum_i R_i^2 - \frac{rbk(k+1)^2}{4}\}}{\sum_{i,j} r_{ij}^2 - \frac{bk(k+1)^2}{4}}$$

in which r_{ij} is the rank of treatment i on block j, each of the b blocks contains k experimental units, each of the t treatments appears in r blocks, and every treatment appears with every other treatment precisely λ times; $n = bk = rt$. Now E[R_i] = $r(k + 1)/2$, $T = \sum_{i,j} r_{ij} = bk(k+1)/2$, $n_{i.}$ = r, $Tn_i/n = (bk/t)(k+1)/2 = r(k+1)/2$, $b_j = k$, $\sum_i r_{ij} = k(k+1)/2$ and

$$kS_j = \{\sum_i r_{ij}^2\} - k(k\ +\ 1)/2)^2.$$

Also

$$\sum_i (R_i - Tn_{i.}/n)^2 = \sum_i (R_i - r(k+1)/2)^2 = \sum_i R_i^2 - \frac{rbk(k+1)^2}{4}.$$

Thus

$$G_{WB} = \frac{k\sum_i R_i^2 - \frac{rbk(k+1)^2}{4}}{r\left\{\sum_{i,j} r_{ij}^2 - \frac{bk(k+1)^2}{4}\right\}} = (h_1^{\text{T}}Z)^2 + \cdots + (h_{t-1}^{\text{T}}Z)^2$$

and

$$D_A = \frac{r(t-1)}{k} G_{WB}.$$

As before, since $h_u^{\mathrm{T}}Z$, $u = 1, \ldots, t-1$ are orthonormal contrasts whose sum of squares is G_{WB}, $h_u^{\mathrm{T}}Z\sqrt{\frac{r(t-1)}{k}} = h_u^{\mathrm{T}}Z\sqrt{\frac{b(t-1)}{t}}$, $u = 1, \ldots, t-1$ are orthonormal contrasts whose sum of squares is D_{A}.

The decomposition for the randomised block design is a particular case of the balanced incomplete block design with $k = t$.

Latin Square Design

If r_{jk} is the overall rank of the observation in row j and column k and $\mu = (t^2 + 1)/2$, then the test statistic, applied at the end of section 1, is

$$RL_{\mathrm{A}} = \frac{\sum_i (R_{i..} - t\mu)^2}{\{\sum_{j,k} r_{jk}^2 / t\} - t(t^2+1)^2/4}.$$

See Livingston and Rayner (2022) and Rayner and Livingston (2022). The rank sum is $T = 1 + \ldots + t^2 = t^2(t^2 + 1)/2$, $n_i = t$ for all i, $n = t^2$, $Tn_i/n = t(t^2 + 1)/2 = t\mu$ and $G_{\mathrm{O}} = \sum_i (R_i - Tn_i/n)^2/(n_i\, var) == (h_1^{\mathrm{T}}Z)^2 + \cdots + (h_{t-1}^{\mathrm{T}}Z)^2 = RL_{\mathrm{A}}$ on substitution. The $h_u^{\mathrm{T}}Z$, $u = 1, \ldots, t-1$ are orthonormal contrasts whose sum of squares is RL_{A}.