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A note on the analysis of difference patterns - structural zeros by design

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Abstract

The method of finite differences is popular in the analysis of series of measures, because it allows one to analyze the shape of the curve that describes the series, and changes in the shape. In addition, it allows one to relate these changes to covariates. In the analysis of categorical variables, researchers can cross the sign patterns of first, second, and higher differences. In this note, it is shown that crossing sign patterns from different levels results in contingency tables with systematically large numbers of structural zeros. In addition, a simple algorithm is proposed that allows one to identify impossible combinations of sign patterns. Examples are presented using empirical and random number-generated data that are analyzed using log-linear models and Configural Frequency Analysis.

Key words: series of measures; method of differences; signs of differences; structural zeros; log-linear modeling; Configural Frequency Analysis

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In behavioral research, measurement and analysis of change are of importance in many contexts. For example, intervention and therapy are concerned with changes in behavior over time. This applies accordingly to prevention and education. The number of methods of analysis of change is large. Among these, the *method of finite differences* plays a prominent role. It can be used for a number of important purposes. The following five applications are most prominent. First, the method allows one to determine a polynomial function that either fits or sufficiently approximates a series of values (for a description of this technique, see Zurmühl, 1965; for applications, see von Eye, 2002). Second, it allows one to identify and correct errors in a series of measures (Hermite interpolation; see, e.g., Zurmühl, 1965). Third, the method can be used to devise numerical solutions of partial differential equations (Smith, 1986). Fourth, the method has been used in the context of modeling. McArdle and collaborators (McArdle, 2001; McArdle & Hamagami, 2001) have devised structural models of developmental change that are based on latent first difference scores. Fifth, the method has been used to describe the shape of trajectories over time (Krauth,1973; Lienert & Krauth, 1973 a, b). The present note is concerned with characteristics of the patterns that result when the signs of the differences are used. That is, this note examines the method of differences in the context of categorical data analysis. Specifically, (1) it will be shown that, when differences of various orders are categorized, the resulting cross-classifications contain structural zeros by design (that is, cells that, by definition, cannot contain any cases), and (2) an algorithm will be presented that allows one to identify those patterns that are structural zeros. Effects of these structural zeros include constraints when it comes to modeling the resulting cross-classifications or performing configural analyses.

1. The method of differences

There exist many variants of the method of finite differences (see Zurmühl, 1965). Here, we use the *method of finite ascending differences* (MFAD) as an example. The following arguments apply accordingly to any of the methods of differences. Consider a series of I measures, X, with values x_i and $i = 1, ..., I$. Then, the MFAD creates *first differences* as $\Delta_{1,j} = x_{j+1} - x_j$, for $j = 1, ..., I - 1$, *second differences* as $\Delta_{2,k} = \Delta_{1,k+1} - \Delta_{1,k}$, for $k = 1, ..., I - 2$, and so forth. If a series of measures can be described using a polynomial of lth order, with $l \leq I - 1$, the lth differences are constant, and all higher-order differences are zero. Consider the data example in Table 1. The table shows, in the second line, the values of the 3rd-order polynomial $y = 25 + 3x + 2x^2 + 0.6x^3$, for values of X from 0 to 6, in steps of 1. In the following rows, it shows the first, second, and higher differences. Obviously, the third differences are constant, and the fourth differences are zero.

Table 1:
First and higher differences for series of six values for the polynomial
$y = 25 + 3x + 2x^2 + 0.6x^3$

X	0	1	2	3	4	5	6
f(X)	25	30.6	43.8	68.2	107.4	165	244.6
Δ_j	5.6	13.2	24.4	39.2	57.6	79.6	
$\Delta_{2,k}$	7.6	11.2	14.8	18.4	22		
$\Delta_{e,l}$	3.6	3.6	3.6	3.6			
$\Delta_{4,m}$	0	0	0				

Figure 1 displays the series of the raw scores (circles), first differences (x symbols), second differences (+ signs), and third differences (triangles). Clearly, with increasing order, the differences become smaller.

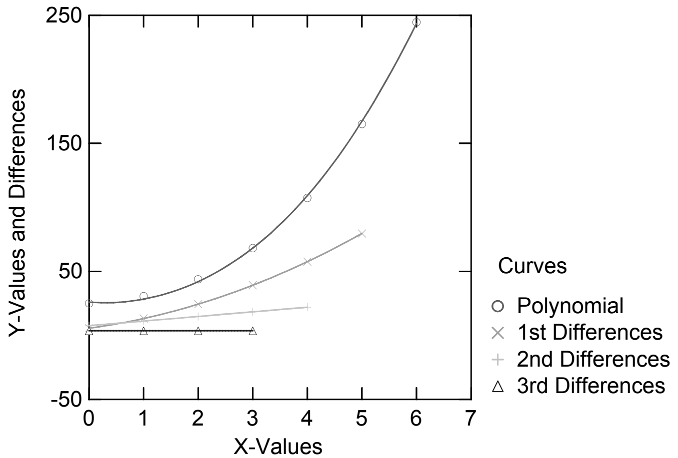

Figure 1:
First and higher differences for a third order polynomial

2. Patterns of differences

In the analysis of empirical data, the numerical value of differences itself often is either not interpretable, e.g., when ordinal scales are used, or not of interest. Instead, researchers may ask whether change is positive ($\Delta > 0$) or negative ($\Delta < 0$)[2]. To analyze patterns of positive and negative change, differences of any order are sign-transformed such that:

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[2] For the following considerations, we will not consider the case in which $\Delta = 0$. However, the following arguments apply accordingly to this case.

$$\operatorname{sgn}\Delta = \begin{cases} 0 & \text{if } \Delta \le 0 \\ 1 & \text{if } \Delta > 0 \end{cases}$$

(Lienert & Krauth, 1973 a, b). Alternative transformations have been discussed (for an overview, see von Eye, 2002).

Now, in the analysis of repeated observations, researchers often ask questions concerning change patterns. To perform analyses, researchers cross the signed variables. That is, variables indicating first and higher differences are crossed.

Data example. For the following example, we use data from a study on the development of aggression in adolescents (Finkelstein, von Eye, & Preece, 1994). In this study, 38 boys and 76 girls in the UK were asked to respond to an aggression questionnaire in 1983, 1985, and 1987. The average age at 1983 was 11 years. One of the dimensions of aggression examined in this study was Physical Aggression against Peers (PAAP). In the present example, we analyze the development of PAAP from 1983 to 1987.

In the present example, a single variable is observed three times. For this series of measures, two indicators of first differences can be created ($\Delta_{1,1}$ = Time 2 - Time 1, and $\Delta_{1,2}$ = Time 3 - Time 2) and one indicator of second differences ($\Delta_{2,1} = \Delta_{1,2} - \Delta_{1,1}$). Each of these indicators is sign-transformed as described above and, thus, dichotomous. Crossed, these three indicators span a 2 x 2 x 2 contingency table. This table has the cell indices 000, 001, 010, 011, 100, 101, 110, and 111. Table 2 displays this cross-classification for the present sample data. In a first analysis, we perform a first order Configural Frequency Analysis (CFA) which uses the log-linear main effect model for a base model (for a discussion of CFA base models, see von Eye, 2004). For the CFA, the z-test was used, and the Bonferroni-adjusted $\alpha^* = 0.00625$.

The log-linear main effect fails to describe the data well. It comes with the LR-X^2 = 81.27 which suggests significant model - data discrepancies ($df = 4$; $p < 0.01$). Indeed, the CFA suggests that two types (over-frequented cells) and two antitypes (under-frequented

Table 2:
CFA and log-linear analysis of first and second differences of Physical Aggression against Peers, observed three times

Configuration[a]	m_{ijk}	$\hat{m}_{ijk}$	z	p	Type/Antitype?
000	25	27.622	-.499	.30892591	
001	21	21.580	-.125	.45034337	
010	0	12.238	-3.498	.00023422	Antitype
011	25	9.561	4.993	.00000030	Type
100	33	16.729	3.978	.00003474	Type
101	0	13.069	-3.615	.00015012	Antitype
110	6	7.412	-.518	.30206214	
111	4	5.790	-.744	.22844302	

[a] The first two digits indicate the first differences (linear changes), the third digit indicates the second differences (quadratic changes); m_{ijk} indicates the observed frequencies for Cell *ijk*, and $\hat{m}_{ijk}$ indicates the estimated expected frequencies for Cell *ijk*.

cells) exist. The first type is constituted by Configuration 011. This pattern describes an initial decrease in physical aggression that is followed by an increase. This pattern has a positive quadratic trend as is indicated by the ‘1’ for the second difference. The second type, constituted by Configuration 100, shows just the opposite curvature. It describes an initial increase that is followed by a decrease in physical aggression. It thus has a negative quadratic trend, indicated by the ‘0’ for the second differences.

The two antitypes are most interesting for the present purposes. The first indicates that not a single adolescent showed a decrease that is followed by an increase and, overall, a negative quadratic trend (Configuration 010). The second indicates that no one showed an initial increase, followed by a decrease in tandem with an overall positive quadratic trend (Configuration 101). It only makes sense that nobody showed these patterns. The first antitype would be a ∪-shaped curve that is, simultaneously, ∩-shaped. The second antitype would be a ∩-shaped curve that is, simultaneously, ∪-shaped. Neither is logically possible. Because of this pattern of contradictory shapes, the cells 010 and 101 must be declared structural zeros.

The effort to fit a standard hierarchical log-linear model, under consideration of the two structural zeros, to the cross-classification in Table 2 is futile. Without the two structural zeros, the hierarchical model with all two-way interactions would have described the data close to perfectly (LR-X^2 = 0.31; df = 1; p = 0.58). However, this model assigns expected frequencies for the cells with structural zeros. Taking into account the structural zeros does not lead to a fitting model that is more parsimonious than the saturated model. More specifically, declaring cells 010 and 101 structural zeros has the effect that the log-linear model with all two-way interactions is left with no degrees of freedom. Removing any of the two-way interactions leads to 1-df models, none of which fits. Therefore, we now recalculate the CFA after declaring these two cells structural zeros. The results of the CFA appear in Table 3. For this CFA, the z-test and the first order base model were used again. However, the Bonferroni-adjusted α^* is now less extreme (α^* = 0.0083) because six instead of eight significance tests are performed.

Table 3:
CFA and log-linear analysis of first and second differences of Physical Aggression against Peers, observed three times; structural zeros taken into account

Configuration[a]	m_{ijk}	$\hat{m}_{ijk}$	z	p	Type/Antitype?
000	25	30.784	-1.042	.14859511	
001	21	26.406	-1.052	.14639006	
010	0	-	-	-	
011	25	13.810	3.011	.00130113	Type
100	33	21.810	2.396	.00828479	Type
101	0	-	-	-	
110	6	11.406	-1.601	.05471897	
111	4	9.784	-1.849	.03221839	

[a] The first two digits indicate the first differences, the third digit indicates the second differences (quadratic changes)

As in the first analysis, the first order CFA main effect base model fails to describe the data well (LR-X^2 = 22.12; df = 2; p < 0.01), and we obtain two types. These types are the same as in Table 2. What used to be antitypes are now structural zeros, with zero probabilities.

In the next section, we discuss the problem with impossible shape patterns in more detail.

3. Structural zeros by design

The following considerations are based on the connection between the method of differences and polynomials. Consider the polynomial of order n,

$$F_n(x) = a_0 + a_1 x + a_2 x^2 + \ldots + a_n x^n = \sum_{i=0}^{n} a_i x^i ,$$

where the a_i are the unknown polynomial coefficients, and x is the variable used to predict the dependent measure. The orientation of a polynomial is determined by the sign of the last non-zero coefficient. For example, in a regression line, the sign of the regression parameter indicates whether the orientation is positive (line has positive slope) or negative (negative slope). This applies to polynomials of any order. Consider, for example, the polynomial $y = 4 + x + 2x^2 + .25x^3$. The left panel of Figure 2 displays this polynomial. The right figure displays this polynomial after the sign of the last term was changed to be negative.

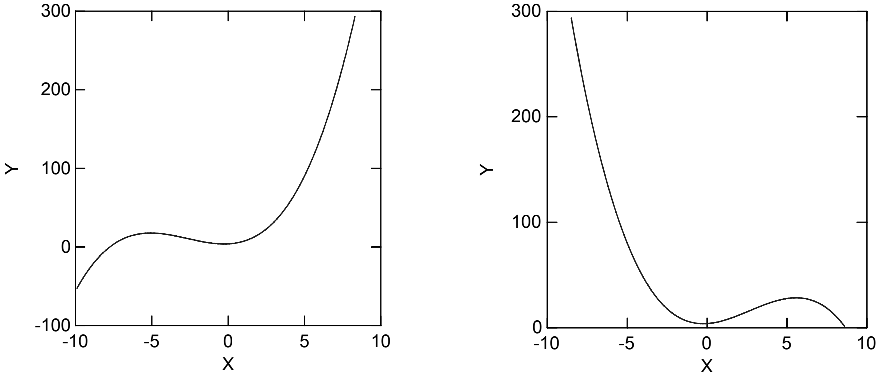

Figure 2:
Polynomial $y = 4 + x + 2x^2 \pm .25x^3$

Clearly, the orientation of the polynomial in the left panel (last coefficient positive) is positive, and the orientation of the polynomial in the right panel (last coefficient negative) is negative. Now, for the following considerations, we use the fact that the signs of differences also indicate the orientation of a polynomial. Consider the polynomial in the left panel. Calculating the difference between the last and the second-last y-values yields a positive score, indicating that the orientation of the curve is, at the end of the series of measures, positive. Accordingly, the difference between the last and the second last y-values in the right panel yields a negative score, indicating that the orientation of the curve is negative. This applies to first differences as well as differences of any order. In addition, this applies to any of the differences within a series, because first differences correspond to first derivatives.

Now, in the application of the method of differences in the context of categorical variable analysis, researchers can cross sign patterns from differences of different orders, thus analyzing the linear, quadratic, cubic etc. elements of series of measures simultaneously. This strategy has the effect that all possible combinations of sign patterns are included in the analysis. Unfortunately, as was illustrated in the last section, all impossible combinations are included also.

Definition: Combinations of sign patterns are impossible if lower-order and higher-order signs suggest different orientations of a series of measures.

This applies to patterns of difference signs of any order. We now ask how to detect impossible sign patterns. To answer this question, we propose an iterative procedure in which all candidate patterns for contradictory description of orientation are examined. Candidates are all sign patterns that indicate a change in orientation (from + to - or vice versa). Patterns that show constant signs do not need to be considered. Now, let $\Delta_{1,j}$ and $\Delta_{1,j+1}$ be the first differences between the adjacent measure pairs x_{j+1} and x_j, and x_{j+2} and x_{j+1}, respectively, for $j = 1, ..., I-1$, and $\Delta_{2,k}$ the corresponding second difference, that is, $\Delta_{1,k+1} - \Delta_{1,k}$. Let sgn $\Delta_{1,j}$, sgn $\Delta_{1,j+1}$, and sgn $\Delta_{2,k}$ be the signs of these differences.

Step 1: Compare each pair of sgn $\Delta_{1,j}$ and sgn $\Delta_{I,j+1}$ with the corresponding sgn $\Delta_{2,k}$. If both sgn $\Delta_{1,j} \neq$ sgn $\Delta_{1,j+I}$ and sgn $\Delta_{1,j+1} \neq$ sgn $\Delta_{2,k}$, then the pattern is impossible. For example, if the sign pattern "+-" at a given difference level is combined with sign "+" at the next higher level, the sign pattern is impossible. The first differences would indicate a negative orientation, whereas the second difference would indicate a positive orientation. Accordingly, the sign pattern "-+" at a given level cannot be combined with the sign "-" at the next higher level. If a sign pair is classified as impossible, proceed to the next sign pattern. If a sign pattern is impossible, all other patterns that could be combined with the impossible pattern are impossible also.

Step 2: Proceed to the next pair of signs, and start over, at Step 1. Continue until all patterns of signs are completed.

This procedure can be applied to sign patterns of all levels. If a researcher decides to skip levels, the procedure can be adjusted. For example, pattern "+-" at level k cannot go with the sign "-" at level k+2. For example, assuming k indicates first differences and $k + 2$ indicates third differences, the sign pattern "+ - +" for first differences and "+" for third differences would indicate the trends depicted in the left panel of Figure 2. For x-values of -10, -5, 0, and 5, the left panel in Figure 2 results in the sign pattern "+ - +" for the three first differences, "- +" for the two second differences, and "+" for the sole third difference. The first signs indicate an initial increase that is followed by a decrease, and then an increase. The second differences signs indicate that the rate of change is initially decelerated and, in later phases, accelerated. The third difference indicates an increase in acceleration. In contrast, consider the series 9, 15, 10, 6. For this sequence, the first differences sign pattern is "+ - -", the second differences sign pattern is "- +" and the corresponding third difference has the sign "+", thus indicating a ∩-shaped trend. For this series, a negative sign for the third difference would be impossible.

In the following example, we analyze an artificial data set. Four random variates (say, a time series of four scores) were created using SYSTAT's uniform random number generator URN. The data set includes 500 cases. Up to third differences can be calculated. For this data set, the three first differences and the two second differences were calculated. None of these was constant, as one would expect from random variates. The differences were transformed into 0 - 1 patterns as described above, with 0 indicating negative or zero differences and 1 indicating positive differences. The resulting dichotomous variables were crossed to span a contingency table with $2^5 = 32$ cells. This table is reproduced in the Appendix. Each of the possible patterns in this table has a frequency greater than 0. Each impossible pattern has a frequency of zero.

To illustrate the algorithm described above, we now ask whether four sample cells in this table are possible, or constitute structural zeros. The results of this analysis are given in Table 4.

Table 4:
Search for structural zeros in a 2^5 cross-classification that is spanned by three first and two second differences

Sign pattern level		Pattern compared		Overall decision for
1^{st}	2^{nd}	1^{st} vs. 2^{nd}		pattern
0 0 0	0 0	0 0 - 0	possible	
		0 0 - 0	possible	possible
0 0 1	0 0	0 0 - 0	possible	
		0 1 - 0	impossible	structural zero
0 0 1	0 1	0 0 - 0	possible	
		0 1 - 1	possible	possible
0 1 1	0 0	0 1 - 0	impossible	structural zero
		1 1 - 0	impossible	structural zero

The rows of the table can be read as follows. From the first sign pattern (left column), we take the first two entries (e.g., 0 0, in the first row), and compare them to the first entry of the second difference sign pattern (0, in the first row). If the second entry of the first differences is equal to the sole entry of the second differences sign pattern, the shape of the curve is described in a compatible way, and we can move on to the next entries of the same row. In the present case, we compare the second two entries of the first differences sign pattern (0 0), in the first row and compare it with the second entry of the second differences sign pattern (0, in the first row). If these are compatible, we are done with the first pattern and can come to a decision. If all comparisons indicate that these are possible patterns, the entire pattern is possible. If only one pattern is impossible, we have to treat the entire pattern as a structural zero.

Table 4 shows the four decision scenarios that are encountered when deciding whether a sign pattern that includes signs from difference levels k and $k + 1$ must be treated as a structural zero. The first of these scenarios (first pair of rows) involves all zeros at the level of first differences. Whenever the sign pattern at level k is constant, any combination with sign patterns at the $k + 1^{st}$ level of differences is possible (for all possible scenarios of this example, see the Appendix).

The second scenario (second pair of rows) shows that, for some sign patterns, the two comparisons suggest different conclusions. In this case, the *impossible* supersedes the *possible*, and the pattern must be treated as a structural zero.

In contrast, in the third scenario (third pair of rows) all comparisons suggest the same conclusion, although the sign patterns are not constant. In this case, all comparisons show that the pattern is *possible*, and the pattern can contain cases. It should be noted that all comparisons need to be made only if, before the last, there is none that would suggest an *impossible* pattern.

The fourth scenario (fourth pair of rows) shows why this is the case. As soon as a pattern is identified as *impossible*, the following comparisons are unnecessary.

If a pattern is impossible, all following patterns, taking higher order differences into account, will be impossible also. If, however, a pattern is possible, some of the following patterns, taking higher order differences into account, may be impossible nevertheless.

In all, of the 32 cells in the present example, 14 are impossible. The log-linear main effect model (base model for first order CFA) that ignores the structural zeros has 26 degrees of freedom. The model that takes the structural zeros into account has 12 degrees of freedom. Accordingly, also taking the third differences signs into account, yields a table with 64 cells. The main effect model for this table has 57 degrees of freedom when the structural zeros are ignored, and 11 degrees of freedom when the structural zeros are taken into account. That is, this table contains 46 structural zeros.

4. Discussion

The analysis of differences is attractive because it allows one to examine change, and variations in change, in the form of ups and downs in a series of measures, adopting a pattern analysis perspective. Taking higher order differences into account, statements can be made about the shape of the series of measures. In the context of latent variable modeling, second differences have been modeled by Hamagami, McArdle, Nesselroade, Ferrer, and Boker (2003). In addition, indicators of shape can be related to each other as well as to other classification variables or covariates, and variable-oriented and person-oriented analyses can be performed.

The present note shows that, in the complete crossing of sign patterns from different levels of finite differences, a large number of structural zeros will always and systematically result. In many cases, structural zeros are not overly problematic, and standard software (e.g., Lem, Splus, SYSTAT) allows one to take them into account. However, three problems render matters complicated. First, structural zeros almost always lead to incomplete designs. Therefore, the interpretation of log-linear parameters can be complicated (Mair, 2006; Mair & von Eye, in press). Second, the models that can be fitted will have to be far less complex than the number of variables and size of the cross-classification would allow otherwise. This was illustrated in Table 3, above, for which no fitting model was found after the structural zeros were taken into account. Therefore, data analysis, in particular modeling such data, may end up in non-fitting models. Accordingly, not all CFA base models may be possible or admissible. For example, the base model of second order CFA requires that all first order associations be taken into account. If, because of the many structural zeros, the required parameters cannot be estimated, this CFA model cannot be applied.

Matters are complicated further by a characteristic of signs of differences that has been explicated before (von Eye, 2002). Signs of differences come with a priori probabilities that do not necessarily correspond with the marginal proportions. Therefore, if researchers wish to take these a priori probabilities into account, additional vectors need to be included in the design matrix. Each of these vectors costs one degree of freedom. Therefore, the complexity of possible log-linear models or CFA base models is reduced even more, and the option of including covariates becomes increasingly remote.

Another issue inherent in the analysis of difference scores is that differences of raw scores that come with measurement error are often unreliable (Lord, 1963). Von Eye (1982) showed that the reliability is not consistently low. Instead, it varies with (1) the reliability of the individual measures and (2) the retest reliability. In contrast, differences from Rasch-scaled scores and from physiological measures have better characteristics. The same often applies to rank differences.

To conclude, the analysis of cross-classifications of sign patterns that are based on finite differences of different order suffers from problems that are caused by possibly large numbers of structural zeros. Structural zeros and, possibly, taking a priori probabilities into account, constrain the models that can be fit to the data to be rather simple.

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Appendix

Cross-tabulation of three first and two second differences signs (artificial data, 500 cases; all zeros in the table are structural zeros)

T2T1[a]	T3T2	T4T3	S21	S22 = 0	S22 = 1
0	0	0	0	2.000	10.000
			1	6.000	5.000
		1	0	0.000	27.000
			1	0.000	32.000
	1	0	0	0.000	0.000
			1	107.000	0.000
		1	0	0.000	0.000
			1	27.000	31.000
1	0	0	0	30.000	31.000
			1	0.000	0.000
		1	0	0.000	104.000
			1	0.000	0.000
	1	0	0	38.000	0.000
			1	29.000	0.000
		1	0	2.000	8.000
			1	8.000	3.000

[a] T2T1 indicates the sign of the difference between measures T1 and T2, T3T2 indicates the sign of the difference between measures T2 and T3, etc.; S21 indicates the sign of the second difference of T2T1 and T3T2 etc.