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A new concept for the cephalometric evaluation of craniofacial patterns (multiharmony)

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SUMMARY Orthodontists commonly specify the alignment of the teeth and jaws by means of a set of *k* angles and their relationship with each other. Each individual can thus be visualized as a point in *k*-dimensional space. Individuals regarded as having an ideal occlusion and well-balanced face, form a cloud of points that is termed the 'norm' population. Individuals far from the cloud require orthodontic intervention.

In this study, a method is presented—the multiharmony method (MHM), which assists in treatment planning. With multiple regression analysis, the expected value that each angle should take in a norm individual when the remaining angles are given is estimated. The residual difference between the measured angle and its expected value then indicates the deviation from a harmonic appearance in the respective angle.

The MHM was applied to a data set of 134 Korean individuals identified as the norm population (Class I, mean age: 19.6 years) and to 87 patients (Class III, mean age: 21.2 years). From the number and size of the residuals, the two populations could be separated almost completely. Almost all patients showed residuals larger than any residual in the norm population (sensitivity: 99 per cent), whereas 90 per cent of all norm individuals showed no extreme residuals. The MHM can also be used to assist in visualizing different treatment effects, thereby assisting the orthodontist in choosing the best course of treatment for each patient.

Introduction

Orthodontists commonly use angles (e.g. SNA and SNB, Figure 1) and their relationship with each other in order to describe the facial skeletal structures. Basically, mean values with standard deviations (SDs) are used in the cephalometric analysis to describe a norm population. The problem in doing so is that patients are interindividually different and reference points (such as nasion) may vary in their locations, such that angles may differ from the mean, but still be 'harmonious'. For that reason, this approach disregards the complexity of interdependencies of skeletal structures (Schudy, 1963, 1964; Solow, 1980; Bishara and Jakobsen, 1985) and the importance of geometric distortion (Battagel, 1993; Melsen and Baumrind, 1995). Hence, cephalometric norms and standards derived from mean values are not simply applicable to the individual case.

Typically, each individual is associated with measurements in *k* different angular variables. This can be imagined as a point in *k*-dimensional space. In this space, individuals regarded as having an ideal occlusion and a well-balanced face form a cloud of points: 'the norm population'. Individuals far from the cloud require orthodontic intervention.

In order to decide about the diagnosis and the form that treatment should take, it is important to identify the causes, i.e. the directions in multidimensional space, in which an individual deviates from the norm cloud. This requires three steps: first, a description of the location of the norm cloud, of the scale and interdependencies between the *k* variables; second, deviations from the norm cloud should be identified in terms of the original angles, such that possible causes of misalignment can be identified, and finally, possible treatment should be suggested, for example, by visualizing the effects that this treatment has on the relationship between the angles.

In order to answer these questions, several mathematical approaches can be used to describe the position and shape of the norm cloud (McIntyre and Mossey, 2003). For example, principal component analysis (PCA) can extract the principal components of the norm cloud, i.e. the directions with maximum variability. This would allow the restriction of the analysis to a few components, i.e. dimensions. However, in PCA, a principal component will usually be a combination of all original variables and therefore, individuals are no longer expressed in the original angles but in a new co-ordinate system, which is less helpful

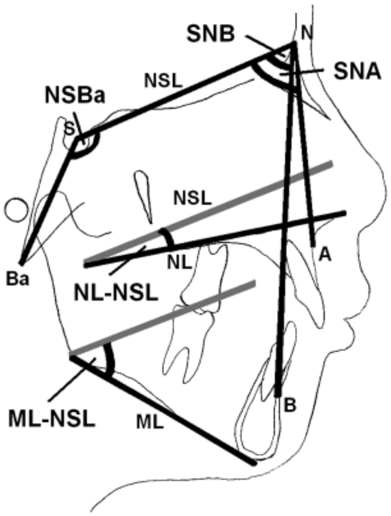

Figure 1 Illustration of the five angles (SNA, SNB, NSBa, NL–NSL, and ML–NSL) used to quantify the alignment of the teeth and jaws.

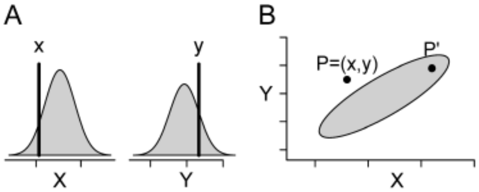

Figure 2 Illustration of the idea that the concept of harmony requires the consideration of relationships between variables. Let *X* and *Y* be two cephalometric angles. If these are positively correlated in the population (cloud of points illustrated in B), an individual with measurements $P = (x,y)$ may appear normal in the univariate representation (univariate distributions illustrated in A) although the relationship between the angles *x* and *y* differs from the normal relationship (B), which can thus not be considered harmonic. *Vice versa*, an individual with extreme measurements $[P' = (x',y')]$ in the univariate representations may still be harmonic if the correlation between its measurements agrees with the relationship in the norm cloud.

in orthodontic practice. Therefore, existing practical approaches rely on methods that can be based on the original set of angles.

The classic angular cephalometric analysis (Steiner analysis), which is widely used in orthodontics (Keim *et al.*, 2002), considers all angles separately (Schwarz, 1926; Downs and Aurora, 1948; Steiner, 1953; McNamara, 1984; McNamara and Ellis, 1988). This analysis is thus based on univariate distributions of the variables (Figure 2A). However, if the norm population shows a specific relationship between the variables, this approach is not sufficient because it disregards the fact that all angles must be in a specific relationship with each other in order to represent a harmonic appearance (e.g. Solow, 1966, see also Figure 2B for a simple example with two variables). In such cases, extreme individual angles can belong to a harmonic constellation (point *P*′ in Figure 2B), whereas intermediate individual angles can belong to an abnormal constellation if their relationship deviates from that in the norm population (point *P*, Figure 2).

Since correlations between angles are essential for the description of a hamonious appearance, the comprehensive analysis regarding floating norms (FN) was introduced by Segner (1989) and Segner and Hasund (1994). Further epidemiological studies have been performed by Hasund and Böe (1980), Järvinen (1986), Tollaro *et al.* (1996), and Franchi *et al.* (1998). This method determines one independent or explanatory variable (usually SNA) and describes its relationship to all other dependent variables as found in the norm population with simple linear regression analysis. These linear relationships then define the size of all other angles that would be expected in a 'harmonic' norm individual. Subjects, regardless as to whether they are orthognathic, retrognathic, or prognathic, can be classified as still harmonious. This definition of harmony will be called floating norm harmonic ('FN-harmonic'). The angles predicted for each SNA value are summarized in a table, called the 'harmony box' (Figure 3A). Deviations from the predictions are quantified with the standard error (SE) derived from multiple linear regression ('harmony scheme', grey area in Figure 3A).

The harmony box has several advantages. First, it takes into account that harmony requires specific relationships between the angles; second, it offers an overview of all measured angles in an individual and indicates when some angles deviate from their harmonic predictions, and finally, the FN method takes into account that there are many potentially harmonious angle combinations, namely all that can be represented in the harmony box on one horizontal line. Thus, if all variables fit the predictor (i.e. SNA), even extreme angles can be considered FN-harmonious.

However, FN-harmony requires only that all variables are in good relation to one predictor. This idea can be useful, but it disregards certain multidimensional relations (Figure 4), so that the diagnosis may not be appropriate. In addition, FN-harmonic angle combinations depend on the chosen independent variable: a harmony box based on SNA differs from one based on SNB (Franchi *et al.*, 1998, see also Figure 3). Finally, the vertical position of the harmony scheme crucially determines which angles are to be considered abnormal in one particular individual (Segner, 1989; Tollaro *et al.*, 1996).

In order to solve these difficulties, it was the aim of this study to develop a method that avoids the problem of predictor choice and that regards the interdependencies of skeletal structures when investigating the agreement between multiple cephalometric angles.

Materials and methods

An approach is presented that is related to the harmony box (Beckmann and Segner, 2002) but avoids the problem of predictor choice by taking into account the multidimensional

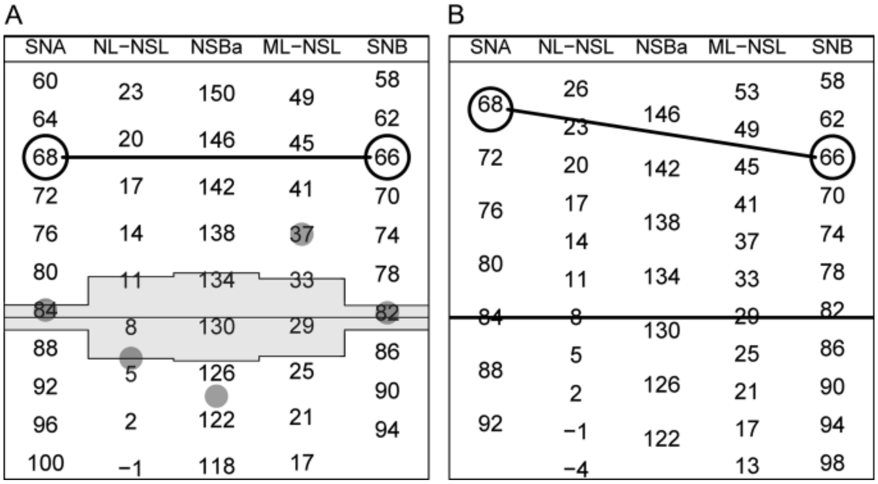

Figure 3 The harmony box as proposed by Segner (1989) derived from the Korean norm population analysed in the present study. (A) For each SNA value, each other angle is predicted with simple linear regression from SNA. Values on a horizontal line are identified as 'harmonic'. The grey area (harmony scheme) represents deviations of ±1 standard errors derived from multiple linear regression. The five angles of an individual are represented as grey points. B: Harmony box derived from the same data set, with SNB as the predictor. For example, the combination SNA = 68 and SNB = 66 is considered harmonious in the analysis based on SNA (A), while SNA = 68 is considered too small as compared with SNB = 66 when basing the analysis on SNB (B).

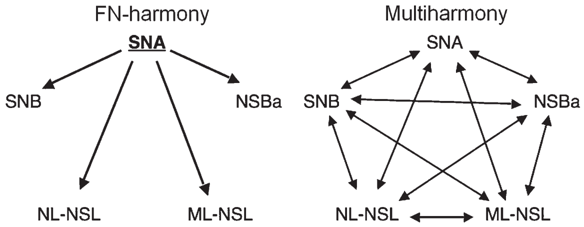

Figure 4 Relationships taken into account by the floating norms (FN) harmony box (left) and by the multiharmony method (MHM; right): FN relates all variables to one pre-identified predictor (here: SNA), while MHM is symmetric in the sense that it relates every variable to all other angles.

relationship between all variables (Figure 4). It is therefore termed the 'multiharmony' method (MHM) and was introduced in detail by Bingmer (2008). The MHM defines a set of angles as multiharmonic if every angle corresponds to its prediction derived from all other angles with multiple linear regression. The difference between the predicted and the observed value in angle *i* then indicates potential abnormalities in this angle.

The approach was applied to a data set of 134 young Korean adults (70 males and 64 females, mean age 19.6 years) that had not received orthodontic treatment. They were selected from students enrolled at Yonsei University Dental Hospital, Seoul, Korea. The subjects had an ideal or near-ideal occlusion (Class I molar and canine relationship, normal overbite and overjet, not more than 3 mm of crowding or 1 mm of spacing, and no missing teeth) and a well-balanced face (Park *et al.*, 1989; Kao *et al.*, 1995; Baik *et al.*, 2000).

The method was also applied to 86 prognathic patients (46 males, mean age 21.7 and 40 females, mean age 20.6 years) diagnosed with a skeletal Class III malocclusion and treatment planned for orthognathic surgery at Yonsei University. The classification was based on pre-treatment cephalometric radiographs using the Segner/Hasund analysis (Segner and Hasund, 1994) and an individualized composite analysis (Ricketts, 1957; Steiner, 1959; Jarabak and Fizzell, 1972; Hasund and Böe, 1980).

The following measurements were carried out using an orthodontic diagnostic software program (FRWin; Computer konkret, Falkenstein, Germany; Figure 1): SNA, SNB, NL–NSL, ML–NSL, and NSBa. All cephalometric radiographs of the two groups were taken with the same device (Cranex 3+Ceph; Soredex, Schutterwald, Germany). The amplification factor was 1:1.1.

Deviations in multiple dimensions

In order to describe the multivariate relationship between the angles in the norm population, multiple linear regression was used: Let $X_i = (x_{1i}, \ldots, x_{ni})$ denote the observations of all *n* norm individuals in angle *i*. Then the 'harmonic' value $\hat{X}_i$ of angle i is estimated from all other angles $X_1, \ldots, X_{i-1}, X_{i+1}, \ldots, X_k$ with multiple regression:

$$\hat{X}_i = b_{i,0} + b_{i,1}X_1 + \cdots + b_{i,i-1}X_{i-1} + b_{i,i+1}X_{i+1} + \cdots + b_{i,k}X_k, \quad i = 1, \ldots, k. \tag{1}$$

Thus, the coefficients $b_{i,0}, \ldots, b_{i,k}$, $i = 1, \ldots, k$, which describe the multivariate relationship, that are perceived as normal are estimated from the norm population.

In the second step, the system of equation (1) is used as a reference for additional individuals Y with measured angles (y_1,..., y_k) as follows: for each angle i, the value $\hat{y}_i$ that would be expected in a norm individual with values $y_1, y_2,..., y_{i-1}, y_{i+1}, ..., y_k$. is predicted by (1):

$$\hat{y}_i = b_{i,0} + b_{i,1}y_1 + \cdots + b_{i,i-1}y_{i-1} + b_{i,i+1}y_{i+1} + \cdots + b_{i,k}y_k .$$

The residual

$$r_i := y_i - \hat{y}_i, \quad i = 1, \ldots k,$$

i.e. the difference between the predicted and the observed size of the angle, indicates potential abnormalities in angle i.

Applying this procedure to all k angles yields k residuals, which can be visualized in a 'residual plot' (Figure 5), a specific type of parallel co-ordinate plot (Inselberg and Dimsdale, 1990). In this representation, each column shows one angle (SNA, NL–NSL, . . .). The ordinate of a point represents the size of the residual in that specific angle: if it is located close to zero (e.g. the black point in column NL–NSL in Figure 5), this indicates a small residual, i.e. the observed angle NL–NSL agrees closely with the value that is predicted from the other angles (SNA, NSBa, ML–NSL, and SNB). A large residual (e.g. the black point in column ML–NSL in Figure 5) indicates potential abnormalities in angle ML–NSL.

In order to determine whether a large residual indicates an abnormal deviation, its size r_i is compared with the residuals obtained for all individuals in the norm population (grey points in Figure 5). An extreme residual, i.e. a value larger than any residual obtained in the norm population, can indicate a potential need for treatment.

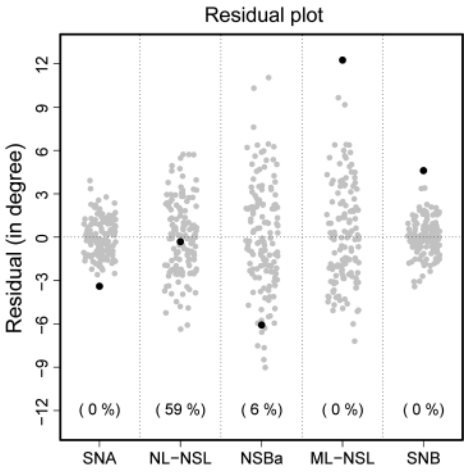

Figure 5 Residual plot. Grey = residuals of norm individuals derived from multiple linear regression. For improved visibility, the points are scattered horizontally. Black = residuals of a patient. Percentages in brackets indicate the number of norm individuals with larger residuals in this angle (0 per cent: extreme residual).

Visualization of treatment objectives

With the aid of the residual plot, whether a potential treatment will result in a multiharmonious angle combination can be investigated. In addition, the approach can suggest several possible treatment options and show whether a change in a single angle might represent sufficient adjustment.

The residual plot can be used in order to visualize the effect of a potential treatment (Figure 6). A patient's angle combination is shown as large triangles, and the effect that treatment of SNB (Figure 6A) or ML–NSL (Figure 6B) would have on the representation of this patient in the residual plot is shown by the smaller triangles. It can be observed that a reduction of SNB of less than 5 degrees yields a representation in which all residuals move into the grey norm clouds, indicating that the respective change might result in potentially successful treatment. In contrast, a change in ML–NSL by as much as 9 degrees can only move the SNA and SNB residuals to the border of the norm cloud.

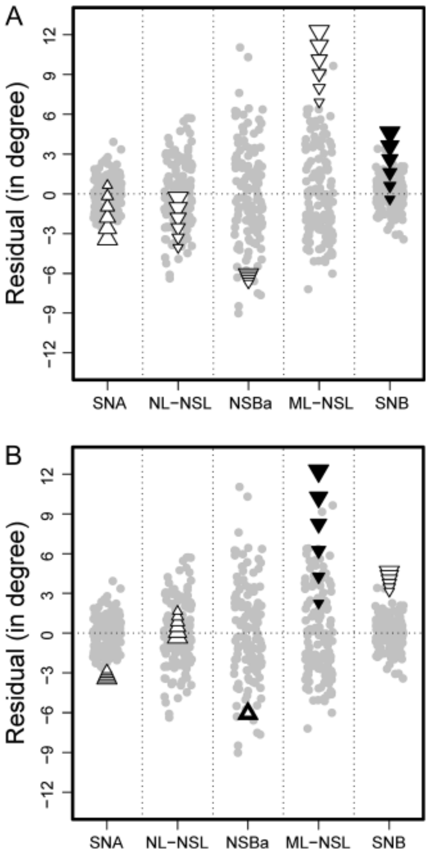

Figure 6 Use of the residual plot to determine the effect of changes in individual angles. Large triangles show the original measurements for one patient. Smaller triangles indicate representations after changing SNA (A) or ML–NSL (B).

It should be noted that a change in a single variable affects the residuals of all angles. This can be explained as follows: if the value X_{SNB} of SNB is reduced and all other variables are kept constant, then the prediction $\hat{X}_{\mathrm{SNB}}$ of SNB does not change, but the residual $r_{\mathrm{SNB}} = X_{\mathrm{SNB}} - \hat{X}_{\mathrm{SNB}}$ will be affected. For all other residuals, e.g. SNA, the value X_{SNA} is kept constant, but the prediction $\hat{X}_{\mathrm{SNA}}$ is affected by a change of SNB, yielding a new residual. The formal terms and relationships are given in Appendix 1. In other words, a change in angle *j* by δ affects the *j*th residual by the same amount. The new residual of any other angle *i* is changed by $-b_{ij}\delta$, where $-b_{ij}$ is the size of the respective multiple regression coefficient in (1).

In addition, the MHM allows direct computation of one specific set of changes in all angles when one is able to pre-specify a particular set of residuals that are to be obtained. The details on this technical method can be found in Appendix 2.

Results

In order to investigate the diagnostic usefulness of the MHM, it was applied to two populations of 134 norm individuals and 86 patients. When performing the analysis for a norm individual, that observation was first excluded from the norm population, and the multiharmonious relationship (1) was then derived from the remaining population before drawing the residual plot of this individual. With this procedure, 121 of 134 norm individuals yielded no extreme deviation, i.e. no residual larger than any other residual occurring in the remaining norm population (specificity: 90 per cent). Of the 134 norm individuals, only 13 had extreme residuals, 11 showing deviations only in one angle (Table 1). For the patient population, all but one showed extreme residuals, and 89 per cent of all patients had extreme deviations in at least two angles (sensitivity: 99 per cent, Table 1).

In comparison, when the harmony box was also applied to the same data set, all patients showed at least one angle outside the harmony scheme (sensitivity: 100 per cent, Table 1). However, since this harmony scheme only allows deviations of 1 SE, as many as 100 (75 per cent) individuals from the norm population also showed angles outside the scheme (specificity: 25 per cent, Table 1).

Thus, the MHM demonstrated a high sensitivity and specificity with the existence of extreme residuals. When taking into account the size of the deviation from the most extreme individual, it was also found that such deviations were considerably larger in the patient than in the norm population (Figure 7A): deviations of norm individuals, if they occurred at all, were observed in all angles and ranged up to 0.4 SE of the linear regression, with an absolute mean of 0.2 SE. In contrast, deviations of patients had an absolute mean of 2 SE and ranged up to 7.8 SE (Figure 7B).

In summary, the number and size of the deviations from the most extreme norm observation could provide strong evidence of a potential need for treatment in the given data set. In addition, the shape of the patient's residuals showed a typical Class III profile, in which SNA was too small relative to SNB (Figure 7A).

Table 1 Number of angles with extreme residuals in the norm and patient population for the defined multiharmony (MH) and floating norms (FN).

	No. of angles with extreme residual	0	1	2	3	4	5
MH	Norm population	121	11	2	0	0	0
	Patient population	1	9	34	33	9	0
FN	Norm population	34	34	38	16	12	0
	Patient population	0	4	27	27	23	5

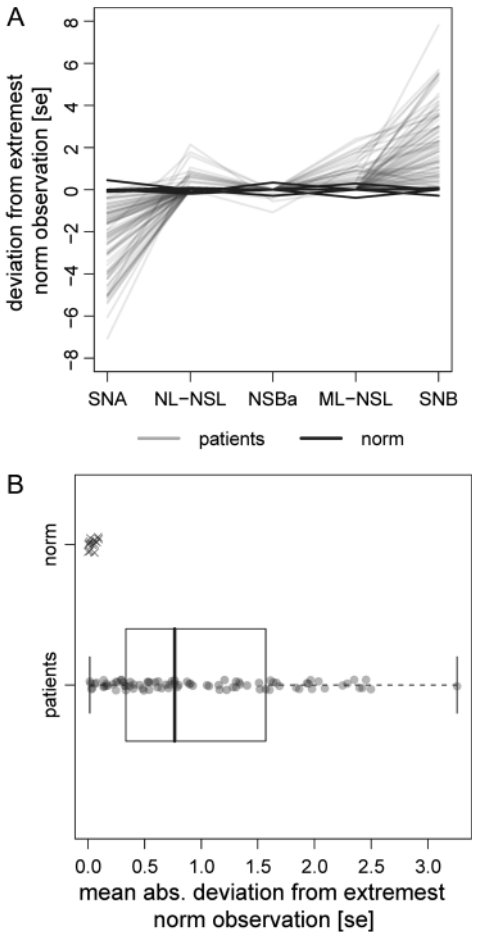

Figure 7 Size of deviations from the most extreme norm observation in the two populations. (A) Profile across all angles, norm (black), and patients (grey) indicates little or no extreme residuals for the norm, and large residuals in the patient population, with a typical Class III profile. (B) The mean absolute deviations across all angles are considerably larger for most patients than for the norm individuals.

Discussion

In the present research, a graphical method was developed that provides three tools that may be helpful in the diagnosis of orthodontic patients and in the choice and evaluation of potential treatment (Bingmer, 2008). Firstly, it is necessary to quantify and describe 'norm' faces, i.e. the location, range, and correlation between the angles that are usually perceived as harmonic. Secondly, one should be able to identify deviations from these norm relationships in terms of the original angles, and finally, the method should be able to suggest a potentially successful treatment and to visualize its effects.

In order to answer these questions, the concept of MH was introduced: a combination of angles of the face was considered (perfectly) multiharmonic if every individual angle corresponded to its prediction derived from all other angles with multiple regression. The regression coefficients that quantify multiharmonic relationships were extracted from a predefined norm population. In a second step, a patient's angle combination was investigated by transforming the measurements of the angles into the residuals between the predicted and observed angles. These residuals were then represented in a residual plot. By comparing the residuals of a patient with the cloud of residuals obtained in the norm population, deviations from MH in individual angles can be identified. This can be helpful in the evaluation of a patient's original status, of potential treatment effects, and of the true treatment results. Finally, it can be a useful tool in follow-up studies for the identification of critical developments.

The application of the MHM to the Korean data set indicated a high diagnostic potential of the residual plot (sensitivity: 98.8 per cent, specificity: 90.3 per cent). The number and size of extreme residuals allowed an almost complete separation of the norm and patient population. Furthermore, specific problems such as a Class III malocclusion could be identified by the shape of the residual profile.

Identifying treatment progress with the MHM

Experience in practical orthodontics is one of the most important factors in the prediction of the outcome of treatment. However, the MHM can be a helpful tool in the assessment of a patient's problems and the choice of a suitable treatment.

In the first place, the residual plot can indicate the angles within a patient's profile that show deviations from MH. A patient's initial values are shown in Table 2. In order to map the initial condition, one can represent the patient in the residual plot (Figure 8B). Here, this representation indicates that SNA is too small, whereas SNB and ML–NSL are larger than expected in a norm individual with the same values in the other angles. For orientation, the representation in the harmony box (Figure 8C) and a schematic figure of the constellation of the jaw bones (Figure 8A) are shown.

In order to investigate different treatment effects, the results of changes in individual angles with the help of the residual plot (Figure 9) can be visualized. For example, one could try to change one of the deviating angles, i.e. SNB (A), ML–NSL (B), or SNA (C). Figure 9 indicates that a reduction in SNB by approximately 7 degrees would result in a multiharmonious angle combination (the smallest triangles are inside the norm clouds for all angles). In contrast, reducing ML–NSL alone would not lead to a suitable angle configuration, and the same holds true for an increase in SNA. In both cases, the residual of at least one angle remains larger than all residuals in the norm population.

Table 2 Cephalometric values of a patient before treatment (in degrees).

SNA	NL–NSL	NSBa	ML–NSL	SNB
83.5	6.5	129.2	36.5	90.7

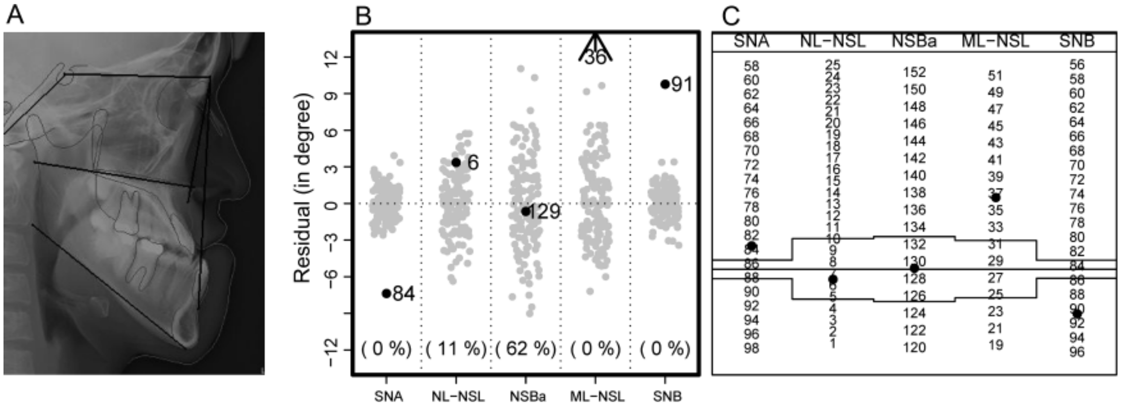

Figure 8 Representation of a patient's initial values. (A) Schematic visualization. (B) Residual plot of the multiharmony method. (C) Harmony box of floating norms. All representations indicate a strong disagreement between SNA and SNB.

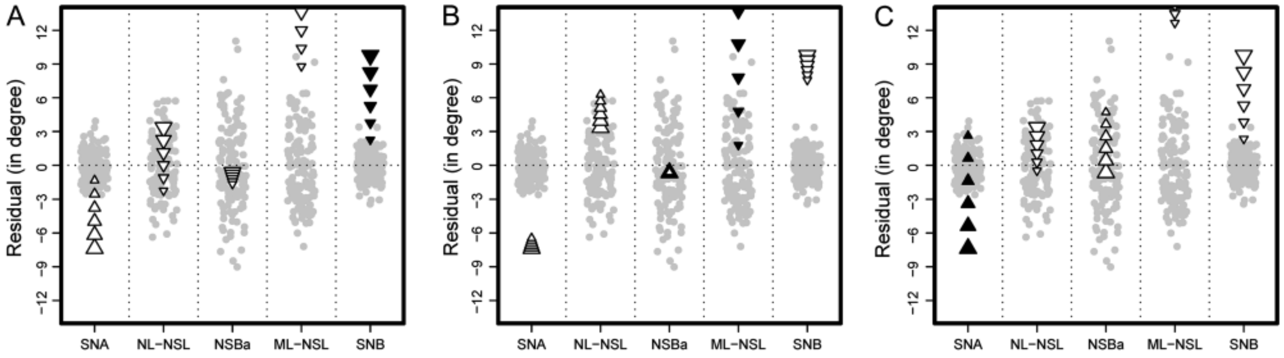

Figure 9 Investigation of three potential treatments with the residual plot: The effects of corrections in the angles SNB, ML–NSL, and SNA are shown in panels (A), (B) and (C), respectively. Triangles are drawn in black for the angle that is varied. Large triangles indicate the initial values of the patient and small triangles the residuals resulting from the corresponding treatment.

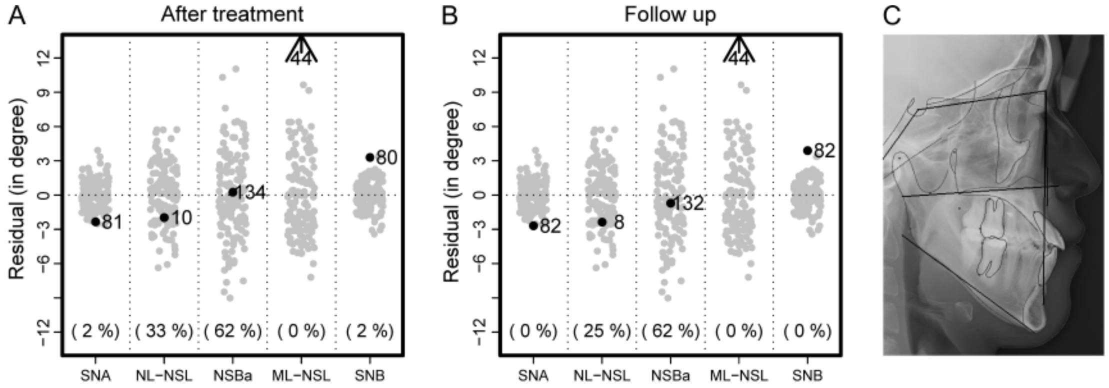

Figure 10 Residual plots of the patient immediately after treatment (A) and in the follow-up period (B). Panel (C) shows a schematic representation of the data in (A).

After treatment, the residual plot can be used to evaluate the resulting angle combination and to track its development during follow-up. The resulting new angle combination can be visualized in the residual plot (Figure 10A). The main change that was observed was a considerable reduction in SNB, and the residual plot indicates that this treatment improved the agreement between the angles: all residuals except ML–NSL could be shifted into the norm cloud. In addition, one can see that slight changes have occurred from Figure 10A (directly after treatment) to Figure 10B (follow-up period). A slight increase in SNB indicates a potentially critical development, pushing the point to the border of the norm cloud.

This indicates that the MHM residual plot can help to map the actual condition of a patient and support the search for successful treatment. In addition, it can be used to evaluate treatment and to trace an individual in the follow-up period. This could be useful in the timely detection of potentially critical developments.

Multiharmony and FN-harmony

As noted, the MHM residual plot and the FN-harmony box presented by Segner (1989) can lead to comparable interpretations of a patient's profile. In general, both approaches are based on linear regression and are thus highly related, particularly near the centre of the norm cloud. Because all regression hyperplanes cross this centre, an observation in the very centre of the norm cloud is perfectly harmonious with both methods (Figure 11A and 11B).

However, there is a conceptual difference between the methods. First, the MHM does not identify one specific predictor but compares every angle with all other angles (Figure 4). As a consequence, the definition of multiharmony is consistent and context-free (Table 3). In contrast, the harmony box requires one angle to be chosen as a predictor and thus the resulting definition of the FN-harmony depends on that predictor. A set of angles that is FN-harmonic when based on SNA will not be perfectly FN-harmonic when based on SNB (unless it is in the centre of the cloud).

This problem is taken into account in the MHM because multiharmony can only be obtained in the very centre of the norm cloud. Outside, at least one angle will show deviations from the prediction. In contrast, many sets of angles can be FN-harmonic, namely, all that are located on a horizontal line in the harmony box. For such a FN-harmonic observation

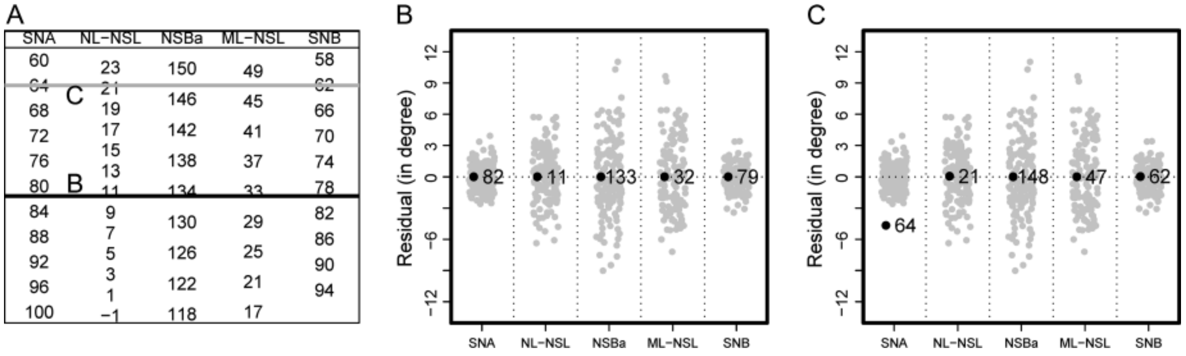

Figure 11 Similarity and differences between floating norms (FN)-harmony and multiharmony (MH). Both methods classify the centre of the mass as harmonious [black horizontal line in A (FN) and zero residuals in B (MH)]. Outside the centre of the mass, all observations forming a horizontal line in the harmony box are FN-harmonic. These are, however, represented in the multiharmony method (MHM) residual plot by $k - 1$ zero residuals and one non-zero residual for the angle that served as a predictor in the harmony box (C), indicating that FN-harmony does not require the predictor to fit the other angles.

Table 3 Comparison of multiharmony and floating norms (FN)-harmony.

	Multiharmony and residual plot	FN-harmony and harmony box
Linear regression	Multivariate	Univariate
Predictors for angle i	All remaining angles	One chosen angle (e.g. SNA)
Harmony	Only in the centre	In the centre and on horizontal lines
—	—	
Interpretation	Context free	Depends on predictor
Sensitivity	99%	100%
Specificity	90%	25%

outside the centre of the mass, the MHM residual plot shows that all angles agree with their prediction except for the predictor in the harmony box (Figure 11C, a rigorous proof of this mathematical relationship can be found in Appendix 3). MH thus contains an additional criterion for harmony. On the other hand, this approach helps to circumvent the problem of predictor choice and thus yields one consistent interpretation. Finally, deviations from perfect harmony that are still considered normal are derived in the MHM from the observations in the norm population. As a consequence, the MHM is able to recognize most norm individuals, while in contrast, 75 per cent of norm individuals show angles outside the FN-harmony scheme.

In addition to these differences between MH and FN-harmony, it should also be noted that the definition of a norm depends crucially on the chosen population (e.g. Hwang *et al.*, 2002). Different populations may differ in the location of individual variables and in the correlations between angles, and they may also show different sizes of variability in faces that are perceived as normal. These differences should be taken into account by adjusting the coefficients in the linear regression separately for each individual population. This can then serve as a reference for patients of that particular population.

Conclusions

The MHM enables the identification of specific variables that show deviations from relationships which would be perceived as normal. In addition, the MHM helps to graphically compare various potential treatments and investigate whether they lead to a multiharmonic angle combination. Although this method is explorative, it can visualize the effects of different treatments in a concise way and thus help to find the most suitable treatment approach for each individual. It is easily implemented on a personal computer.

The presented MHM allows for extensions in various ways. First, it is not restricted to the five variables used. It can easily be applied to a higher number of variables, including angles from 3D facial representations and thus allows for visualizing treatment objectives regarding skeletal and soft tissue changes. Second, one could also combine the evaluation of different treatments with expert knowledge about specific problems and discomfort, allowing for a combination of objective and experience-based criteria. Finally, depending on the intended effect, the graphical representation of the residual plot could also be extended, including for example a graphical indication of extreme residuals or a box that shows the size of a SD, similar to the representation in the harmony box. The MHM can thus serve as a supportive tool for the orthodontic expert in the diagnosis and decision for potential treatment.

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Appendix 1

Treatment effects on the residual plot

For $k = 2$ dimensions the manner in which a set of angles is represented in the residual plot is illustrated. For $k = 2$ angles, (1) reduces to two univariate linear regressions:

$$\hat{X}_1 = b_{10} + b_{12}X_2 \quad \text{and} \quad \hat{X}_2 = b_{20} + b_{21}X_1.$$

The two regression lines (Figure 12A and 12B) differ in slope unless X_1 and X_2 are perfectly correlated. A patient $P = (x_1, x_2)$ (Figure 12A) is then represented in the residual plot with two residuals (circles in Figure 12C)

$$r_1 = x_1 - (b_{10} + b_{12}x_2) \quad \text{and} \quad r_2 = x_2 - (b_{20} + b_{21}x_1). \tag{A.1}$$

Changing x_1 by $\Delta x_1 := x_1' - x_1$ yields new residuals in both variables (P' in Figure 12B, C):

$$r_1' = x_1' - (b_{10} + b_{12}x_2) \quad \text{and} \quad r_2' = x_2' - (b_{20} + b_{21}x_1). \tag{A.2}$$

Thus, the residuals have changed by

$$\begin{aligned} r_1' - r_1 &= x_1' - x_1 = \Delta x_1 \quad \text{and} \\ r_2' - r_2 &= -b_{21}(x_1' - x_1) = -b_{21}\Delta x_1. \end{aligned} \tag{A.3}$$

The same holds true for higher dimensions: the coefficients b_{ij} of the multiple regression determine the amount to which a change in one angle j affects the other residuals r_{i}. If r_i' denotes the new residual in angle i after adjusting angle x_j, the following equation is obtained:

$$r_1' - r_1 = \begin{cases} \Delta x_j & i = j \\ -b_{ij}\Delta x_j & i \neq j. \end{cases} \tag{A.4}$$

Appendix 2

Mathematical derivation of a particular treatment

From (A.4), let

$$M := \begin{pmatrix} 1 & -b_{12} & \cdots & -b_{1k} \\ -b_{21} & 1 & \cdots & -b_{2k} \\ \vdots & \vdots & \ddots & \vdots \\ -b_{k1} & \cdots & -b_{k(k-1)} & 1 \end{pmatrix} \tag{A.5}$$

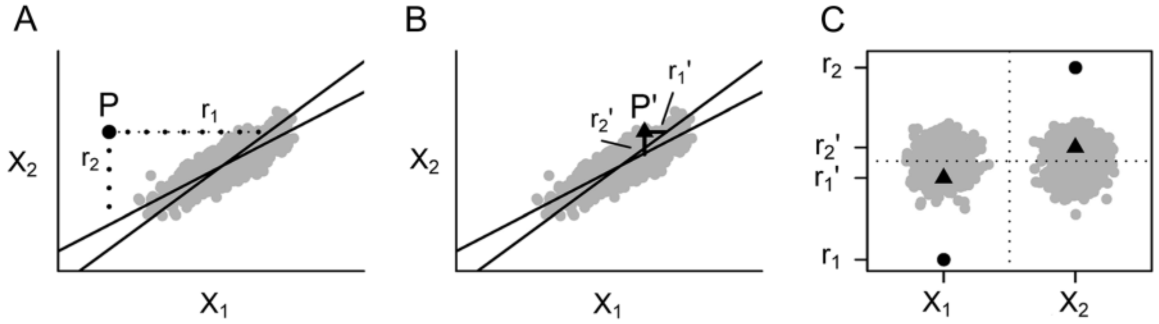

Figure 12 The effect of angle adjustments onto the residual plot in $k = 2$ dimensions. An observation $P = (x, y)$ (A) outside the norm cloud is represented by the residuals in the residual plot [(r_1, r_2), circles in C]. When changing one variable (here: X_1, see B), both residuals are affected [(r_1', r_2'), triangles in C].

denote the matrix of changes in the residuals. If $R = (r_1, \dots, r_k)$ denotes the original set of residuals of a patient and $R' = (r_1', \dots, r_k')$ the pre-specified goal residual vector, the desired treatment can be derived as follows. Let $P = (x_1, \dots, x_k)$ and $P' = (x_1', \dots, x_k')$ denote the original and the new vectors of angles. Then the treatment, i.e. the change in the angles, is denoted by $T = P' - P$. Writing (A.4) in matrix notation yields

$$R' - R = M(P' - P),$$

and if M is invertible, T can be derived by

$$T = P' - P = M^{-1}(R' - R). \qquad \text{(A.6)}$$

Appendix 3

Mathematical relationship between FN-harmony and MH

A FN-harmonic combination of angles outside the centre of mass is represented in the residual plot by $k - 1$ zero residuals and one non-zero residual in the angle that was chosen as the FN-predictor. For reasons of simplicity, the claim is proven for centred vectors, which do not represent a restriction.

Let $X_1, \dots, X_k \in \mathbb{R}^n$ be vectors of n observations (individuals) in k variables (angles). Let X_1 be the angle that is chosen as FN-predictor in the harmony box. Let $a_2, \dots, a_k$ denote the coefficients in the univariate regressions in the FN approach, i.e. they are derived such that

$$a_j = \arg\min \left\| X_j - a_j X_1 \right\|^2 \quad \text{i.e.} \quad \hat{X}_j := a_j X_j = P_{X_1} X_j \quad \text{(A.7)}$$

for $j = 2, \dots, k$. Here, $P_X V$ denotes the orthogonal projection of a vector V onto the linear hull of X. A FN-harmonic constellation can thus be written as $(X_1, \hat{X}_2, \hat{X}_3, \cdots, \hat{X}_k)$, where $\hat{X}_j = a_j X_j = P_{X_1} X_j \quad \forall j = 2, \dots, k$.

In order to show that such a FN-harmonic representation yields zero residuals for all angles $j = 2, \dots, k$ in the MHM, note the following: in the MHM, the prediction of each X_j, $j = 2, \dots, k$, is derived by multivariate linear regression. Thus, the coefficients b_{jl}, $j \neq l$ are estimated such that

$$\sum_{l \neq j} b_{jl} X_l = P_{(X_1, \dots, X_{j-1}, X_{j+1}, \dots, X_k)} X_j. \qquad \text{(A.8)}$$

Theorem Let $X_1, \dots, X_k$, $\hat{X}_2, \dots \hat{X}_k$, $a_2, \dots, a_k$, and b_{jl} $j = 2, \dots, k$, $l \neq j$ be as above. W.l.o.g. let X_1 be the FN-predictor. Then for $j = 2, \dots, k$, the following holds:

$$b_{j1} X_1 + \sum_{l \neq 1, j} b_{jl} a_l X_1 = P_{X_1} X_j,$$

i.e. the univariate FN-prediction of X_j ($P_{X_1} X_j = \hat{X}_j$, right side) equals the multivariate MHM-prediction (left side) of X_j when all angles belong to a FN-harmonic constellation. Thus, all MHM residuals r_j, $j = 2, \dots, k$, are zero in a FN-harmonic constellation based on the predictor X_1.

Proof.

Equation (A.8) and the linearity of orthogonal projection are used, i.e.

$$P_W(V_1 + V_2) = P_W V_1 + P_W V_2 \quad \forall V_1, V_2, W \in \mathbb{R}^n.$$

The proposition then follows directly: for $j = 2, \dots, k$,

$$\begin{aligned}
P_{(X_1, \dots, X_{j-1}, X_{j+1}, \dots, X_k)} X_j &= \sum_{l \neq j} b_{jl} X_l \\
\Rightarrow P_{X_1} X_j = P_{X_1} P_{(X_1, \dots, X_{j-1}, X_{j+1}, \dots, X_k)} X_j &= P_{X_1} \left(\sum_{l \neq j} b_{jl} X_l \right) \\
&= P_{X_1} b_{j1} X_1 + \sum_{l \neq 1, j} P_{X_1} b_{jl} X_l \\
&= b_{j1} X_1 + \sum_{l \neq 1, j} b_{jl} \hat{X}_l.
\end{aligned}$$