Original Article

Shape variation and covariation of upper and lower dental arches of an orthodontic population

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Summary

Objectives: This study aimed to quantify the patterns of shape variability and the extent and patterns of shape covariation between the upper and lower dental arch in an orthodontic population.

Methods: Dental casts of 133 white subjects (61 males, 72 females; ages 10.6–26.6) were scanned and digitized in three dimensions. Landmarks were placed on the incisal margins and on the cusps of canines, premolars, and molars. Geometric morphometric methods were applied (Procrustes superimposition and principal component analysis). Sexual dimorphism and allometry were evaluated with permutation tests and age–size and age–shape correlations were computed. Two-block partial least squares analysis was used to assess covariation of shape.

Results: The first four principal components represented shape patterns that are often encountered and recognized in clinical practice, accounting for 6–31 per cent of total variance. No shape sexual dimorphism was found, nevertheless, there was statistically significant size difference between males and females. Allometry was statistically significant, but low (upper: $R^2 = 0.0528, P < 0.000$, lower: $R^2 = 0.0587, P < 0.000$). Age and shape were weakly correlated (upper: $R^2 = 0.0370, P = 0.0001$, lower: $R^2 = 0.0587, P = 0.0046$). Upper and lower arches covaried significantly (RV coefficient: 33 per cent). The main pattern of covariation between the dental arches was arch width (80 per cent of total covariance); the second component related the maxillary canine vertical position to the mandibular canine labiolingual position (11 per cent of total covariance).

Limitations: Results may not be applicable to the general population. Age range was wide and age-related findings are limited by the cross-sectional design. Aetiology of malocclusion was also not considered.

Conclusions: Covariation patterns showed that the dental arches were integrated in width and depth. Integration in the vertical dimension was weak, mainly restricted to maxillary canine position.

Introduction

Numerous studies have analysed dental arch form in order to assess its role in orthodontic diagnosis and treatment planning (1–3). The dental arch form can influence not only available space, but also dental and smile aesthetics, and potentially long-term occlusal stability (4–7). Furthermore, respecting the pre-treatment dental arch form may help reduce crowding relapse and periodontal damage (5, 8).

Previous efforts to assess dental arch form have described shape by means of conventional biometry, using angles, linear distances, and ratios (1–3, 9). Most researchers have focused on the normal or ideal dental arch and have used algebraic or geometric formulae to describe it. Such geometric figures and mathematical functions, most of which enforce symmetry, include: semicircle (10), ellipse (1, 11), parabola (12), hyperbola (13), catenary curve (14), the cubic spline function (15), conic sections (8,16), polynomial
functions, including the fourth-order polynomial (17, 18) and the sixth-order polynomial (7, 9), Euclidean distance matrices (19), Fourier series (20), and the beta function (3, 9). Mixed models have also been used, such as, ellipse and parabola (21), a semicircle joined to straight segments (10) and a combination of the polynomial, parabola and hyperbolic cosine functions (22). Some of these shapes have formed the basis for deriving commercially produced arch forms (1, 10, 23).

The maxillary and mandibular dental arches reside in the same environment and closely interact with each other for functional occlusion. In a population of normal (close to the ideal) occlusion, high covariation would be expected between the upper and lower arch; one arch would be sufficient to infer the precise position of the teeth of the opposing arch. In contrast, malocclusions show a much wider range of variations in arch form and individual tooth position, and covariation is presumably lower. Which covariation patterns remain strong and which fade away is a question that has not been investigated. Assessing the patterns of covariation in an orthodontic population could reveal which malocclusion features of the upper and lower arch are correlated and expected to co-occur, and which are relatively independent. By extension, covariation could unveil the scope of influence of the aetiological factors that contribute to the various aspects of the malocclusion. Our purpose here was to study 1. the patterns of shape variability in an orthodontic population, indicating the diversity that can be encountered, and 2. the extent and patterns of covariation between the arches. To assess these parameters, we used tools of geometric morphometrics. The presence of sexual dimorphism, allometry, correlation between age–size, and age–shape were also evaluated.

Materials and methods
Sample
Estimating the appropriate sample size in geometric morphometric studies is difficult and guidelines are practically absent in the literature (24). Since we were mainly interested in covariation, we were guided by the results of Fruciano et al. (25), who showed a sample-size effect on the RV coefficient (used to assess covariation strength, see below); samples of small size show inflated RV values, which decrease with increasing sample size and stabilize at sizes above 100, so this was our minimum target size.

The records of the Department of Orthodontics of the School of Dentistry of the National and Kapodistrian University of Athens were searched to select patients for inclusion in this study. The inclusion/exclusion criteria were as follows:

- Permanent dentition; all teeth anterior to second molars present.
- No supernumerary teeth.
- No excessive tooth wear; tooth wear index (TWI) of 0 or 1 (26).
- No congenital malformations, systemic diseases, or syndromic conditions.
- No history of trauma.
- No previous orthodontic or prosthetic treatment.
- No restorations extending to contact areas, cusp tips, or incisal edges.
- No overt crown shape or size abnormalities.

In total, 133 white patients, 61 males and 72 females, fulfilled these criteria. Descriptive statistics of the sample are presented in Table 1. As expected, these subjects presented with a wide range of dental malocclusion patterns and therefore cannot be considered representative of the general population.

<table>
<thead>
<tr>
<th>Table 1. Descriptive statistics of the sample.</th>
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<tr>
<td>Age (years)</td>
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<td>Overjet (mm)</td>
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<td>Overbite (mm)</td>
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<td>Irregularity index (mm)</td>
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<td>Openbite</td>
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The maxillary and mandibular dental casts of each subject were scanned with a structured light 3D scanner (Identica, Medit Co. Ltd, Seoul, Korea). Twenty-two landmarks for the maxillary dentition and 24 landmarks for the mandibular dentition were digitized using the Viewbox 4 software (dHAL software, Kifissia, Greece). The landmarks chosen for digitization were the middle of the incisal edge of the central and lateral incisors, and the cusp tips of canines, first and second premolars, and first molars. Each set of landmarks represented the dental arch form of each jaw in three dimensions (Figure 1).

Geometric morphometrics and statistical analysis
Generalized partial least squares Procrustes superimposition with orthogonal projection on the tangent plane (27, 28) was applied to the landmark sets of each jaw, in order to extract Procrustes coordinates for shape description. The natural logarithm of centroid size (lnCS) was used for size assessment (27, 28).

Principal component analysis
Principal component analysis (PCA) was performed on the Procrustes coordinates to reveal the main patterns of dental arch shape variation (29). In order to determine the number of principal components (PCs) considered as statistically significant, we used three criteria: the broken-stick criterion, rnd-lambda, and the avg-rnd (30). We evaluated as many PCs as specified by at least two of the three criteria.

Shape and size sexual dimorphism
Sexual dimorphism was tested by permutation tests, assessing the Procrustes distance between the mean values of each group in shape space and in form space (i.e. with lnCS included) (31).

Allometry, age–size correlation, age–shape correlation, regression analysis
Multivariate regression analysis was performed to investigate the relationship of shape variables (dependent variables: PCs) on size (independent variable: lnCS). Furthermore, regression analysis was performed to investigate the relationship of age on size, and age on shape.

Two-block partial least squares analysis
Two-block partial least squares (2B-PLS) analysis (32) was performed for the whole sample, as well as for males and females separately, in...
order to investigate any patterns of covariation between upper and lower arch form. The analysis was conducted with MorphoJ software (33) and covariation strength was evaluated by the RV coefficient (34).

We also performed a rarefaction analysis (25), in order to evaluate the effect of sample size on the RV coefficient. Specifically, we created 20 subsamples, each of \(N = 120\), by drawing 120 subjects randomly from the original sample, without replacement. We then computed the RV coefficient for these 20 subsamples and compared the results to those of the original sample. The same procedure was repeated for 20 subsamples each of \(N = 100, 80, 60, 40,\) and 20.

Method error

Twenty scanned dental casts of both jaws were randomly selected and redigitized by the same investigator 10 days after the first digitization. Random error was expressed as the distance between repeated digitizations in shape space compared with the total variance of the sample.

Results

Method error

Mean random error of the 20 repeated digitizations, expressed as a percentage of total shape variance, was 2.39 per cent (range: 1.18–4.66 per cent, SD = 0.81 per cent) and 2.70 per cent (range: 1.01–4.82 per cent, SD = 0.84 per cent), for upper and lower arches, respectively.

Sexual dimorphism and size difference

There was no statistically significant difference in either upper or lower dental arch shapes between males and females (10 000 permutations, upper dental arch form \(P = 0.098\), lower dental arch form \(P = 0.117\)) (Figure 2; Table 2). On the contrary, a statistically significant size difference in both dental arches was found between the genders (Table 3).

Procrustes superimposition and PCA

The first six PCs of the maxillary arch form were considered to be statistically meaningful (70.1 per cent of total shape variance); for the mandibular arch, the first seven PCs were considered to be statistically meaningful (68.8 per cent of total variance) (Table 4). Of the PCs describing upper dental arch form, the first four, accounting for 31.0, 12.9, 9.1, and 7.6 per cent of total variance,
respectively, were found to represent shape patterns that are often encountered and recognized in clinical practice (Figure 3). PC1 described arch width/arc length ratio, PC2 referred to the ectopic position of permanent canines, as far as the vertical plane is concerned. PC3 described the palatal–labial position of central and lateral incisors, and PC4 the arch asymmetry related to the ectopic position of the hemimarch canine in the horizontal plane.

Of the PCs describing lower dental arch form, the first four PCs were also found to represent commonly encountered shape patterns, accounting for 31.5, 11.9, 7.8, and 6.0 per cent of total variance, respectively (Figure 4). PC1 described arch width/arc length ratio, PC2 referred to labial ectopic position of permanent canines, PC3 and PC4 to vertical changes concerning the steepness of the curve of Spee.

Allometry, age–size correlation, age–shape correlation

In form space, PC1 refers mostly to size rather than shape. Thus, any inclination of the vector of pure size change relative to the PC1 axis may indicate the presence of allometry (31). Visual inspection of the form-space plots (Figure 5) indicated allometry, which was confirmed by the results of multivariate regression. Allometry was statistically significant but weak for both the upper and the lower dental arch (upper: $R^2 = 0.05$, $P < 0.000$, lower: $R^2 = 0.06$, $P < 0.000$, 10 000 permutations). A small-sized maxillary arch was related to high position of the canines; as size increases, the canines adopt a normal position within the arch (Figure 6a). Likewise, in the mandibular arch, the position of the canine was mainly related to size, but in the horizontal instead of the vertical plane (Figure 6b).

The correlation between age and shape indicated that the arch width/arc length ratio increased as subjects get older, for both upper and lower dental arches, but the correlation was weak (upper: $R^2 = 0.04$, $P = 0.0001$, lower: $R^2 = 0.06$, $P = 0.005$, 10 000 permutations). A small-sized maxillary arch was related to high position of the canines; as size increases, the canines adopt a normal position within the arch (Figure 6a). Likewise, in the mandibular arch, the position of the canine was mainly related to size, but in the horizontal instead of the vertical plane (Figure 6b).

The correlation between age and size suggested that the size of the dental arch tends to decrease as subjects get older, for both upper and lower dental arch, but this result was not statistically significant (upper: $R^2 = 0.02$, $P = 0.1511$, lower: $R^2 = 0.004$, $P = 0.483$).

Two-block partial least squares analysis

Upper and lower arches covaried significantly (RV coefficient: 33 per cent, Table 5). PLS1 accounted for more than 80 per cent of the total covariance and was related to arch width (Figure 8). PLS2 accounted for approximately 11 per cent of the total covariance and related maxillary canine vertical position to mandibular canine labiolingual position. Similar results were obtained for males and females separately (males: RV coefficient = 0.38, females: RV coefficient = 0.35, $P < 0.0001$). Note that the gender-specific RV values are larger than the value of the total sample. This is a sample size related effect (23).

The rarefaction procedure showed a steady decrease of the calculated RV coefficient as sample size increased from 20 subjects (median RV of 20 samples: 0.48) to 120 subjects (median RV of 20 samples: 0.34). Values reached a plateau at a sample size of 80 (median RV of 20 samples: 0.35).

Discussion

The sample of this study consisted of orthodontic patients, so the outcomes cannot be considered representative of the general population. Nevertheless, the sample included a wide spectrum of different malocclusions and a broad range of arch shape patterns could thus be described. In contrast to most previous studies (see e.g. 1, 11, 17, 23), we did not assume symmetry, either explicitly or implicitly, because our aim was not to describe the average shape but rather to unveil the variability patterns that are inherent in the population.

The choice of landmarks was based on the need to represent the arch form at the occlusal level, where higher correlation between arch forms was expected. Several points were used for the representation of the posterior teeth, thus providing more information about their spatial position and inclination. Other studies have used reference points on the calculated centroids of the occlusal surfaces (35), at contact points (14), at the facial axis point (18, 36), or on glass beads simulating bonded brackets (7).

Table 4. Percent variance described by the first principal components that were considered to be statistically meaningful, in shape space and in form space.

<table>
<thead>
<tr>
<th></th>
<th>Upper dental arch</th>
<th>Lower dental arch</th>
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<tbody>
<tr>
<td></td>
<td>Shape space (%)</td>
<td>Form space (%)</td>
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<tr>
<td></td>
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<tr>
<td>PC1</td>
<td>31.0</td>
<td>38.3</td>
</tr>
<tr>
<td>PC2</td>
<td>12.9</td>
<td>19.8</td>
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<tr>
<td>PC3</td>
<td>9.1</td>
<td>6.0</td>
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<tr>
<td>PC4</td>
<td>7.6</td>
<td>5.7</td>
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<tr>
<td>PC5</td>
<td>5.7</td>
<td>5.0</td>
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<tr>
<td>PC6</td>
<td>3.8</td>
<td>3.3</td>
</tr>
<tr>
<td>PC7</td>
<td>—</td>
<td>3.5</td>
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<tr>
<td>Sum</td>
<td>70.1</td>
<td>78.1</td>
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Results of permutation test for shape sexual dimorphism without replacement (10 000 repetitions).

<table>
<thead>
<tr>
<th></th>
<th>Male group $(n = 61)$</th>
<th>Female group $(n=72)$</th>
<th>% male/female size ratio</th>
<th>$t$ test $t$ (P value)</th>
<th>Permutation test $P$ value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Upper dental arch</td>
<td>4.66 (0.050)</td>
<td>4.62 (0.049)</td>
<td>4.3%</td>
<td>4.86 ($P &lt; 0.0001$)</td>
<td>&lt;0.000</td>
</tr>
<tr>
<td>Lower dental arch</td>
<td>4.62 (0.048)</td>
<td>4.57 (0.044)</td>
<td>5.6%</td>
<td>6.86 ($P &lt; 0.0001$)</td>
<td>&lt;0.000</td>
</tr>
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</table>

Results of $t$ test and permutation test (10 000 repetitions, without replacement) for size sexual dimorphism.
**Shape and size sexual dimorphism**

No statistically significant difference was detected between male and female shape. This is consistent with the results of other studies that used Euclidean distance matrix analysis (37), thin-plate spline analysis (36) and the ninth-degree polynomial function (38). The subjects used in those studies were from southern Europe, as the ones in this study, but they included persons with natural ideal occlusion. Shape sexual dimorphism was also not found in South Australian (39) and Korean populations (40). Regarding size, our male group had approximately five per cent larger upper and lower dental arches than females, in line with other investigators (41).

**Shape and size relation to age**

A statistically significant correlation was observed between age and shape: arch width/length ratio increased with age, for
both upper, and lower dental arches. The correlation was weak, accounting for less than six per cent of the total variance, and was based on a cross-sectional sample, so it should be interpreted with caution. Results from the literature are varied. Studies investigating width changes at ages after the eruption of the second molar, as was our study, showed arch width increase in male subjects and decrease in females (42), decrease in all subjects (43), or slight to no change (44). Longitudinal studies (2, 45) have reported slight increases in arch width, but the changes were subtle and could be easily missed without serial data. A moderate increase in width of the dental arches can be expected, particularly in the anterior regions, until the permanent canines erupt (46, 47). After this time, arch width usually decreases in both the anterior and posterior regions, as does arch length. It is difficult to compare our

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Figure 4. TPS grids depicting the effect of varying each of the four most significant PCs for lower arch form. Each figure presents the deformation at 3 SD in the negative (left) and positive (right) direction. Blue: shape consensus, red: −3SD/+3SD configurations.
results to the above-mentioned studies, because they measured width and length as linear distances, thus potentially confounding shape and size.

We could not detect a statistically significant correlation between age and size. This may appear contradictory to the recognized progressive lower arch crowding but our sample was cross-sectional, was limited in its age range, and the wide intersubject variation in size could have easily overshadowed any size-age correlation. Increased crowding has been reported between the ages of 13 and 18 years (48), between 12 and 21 years (49), 11 and 25 years (50), 13 and 20 years (51), and 13 and 26 years (52).

Shape patterns

The shape variation patterns of the two arches were familiar patterns easily recognized by a clinician. Approximately one-third of shape variation of both arches was related to arch width/length ratio and overall arch shape (triangular versus square). Such high variation questions the clinical practice of using a limited stock of preformed archwires during treatment and emphasizes the need to individualize archwire shape.

The second most significant shape pattern related to canine position, but this was different between the arches: in the maxillary arch, variability was mainly in the vertical direction, whereas in the mandibular arch it was in the horizontal plane. High position of the maxillary canine is a common finding; frequently it is bilateral, but unilateral ectopic canines are also seen. PC2 and PC4 describe both of these cases and covered approximately 20 per cent of maxillary arch shape variability. A smaller percentage was related to incisor position, describing the labiolingual relationship of central and lateral incisors, as is encountered in maloclusions exhibiting a ‘Class II division 2’ incisor pattern. It is interesting to note that vertical discrepancies, apart from canine position, were not represented in the main patterns (PC1–PC4) of the mandibular arch. In contrast, PC3 and PC4 of the mandibular arch were related to the curve of Spee and the related vertical position of incisors and canines.

Shape covariation

The RV value of 33 per cent shows that significant integration between the arches exists, but there is also considerable leeway for independent variability. The main covariation pattern (PLS1, 80 per cent of the total covariation) was related to interarch width. Such a correlation is expected due to a multitude of factors. First, intercusption creates occlusal forces on inclined planes that guide teeth towards a cusp–fossa relationship. It has been suggested that cusps in humans primarily exist to guide teeth into occlusion and may then be disposable, even designed for removal by the forces of attrition (53, 54). A second factor leading to covariation is that both upper and lower arches are part of the oral capsular matrix (55) and are thus influenced by the same functional demands. Muscle development and function are instrumental in determining the growth of the jaws and their final shape and size (56–58). Masticatory muscle thickness shows a significant positive association with maxillary arch width (59, 60), intergonial width and bizygomatic facial width (61). Furthermore, the upper and lower arches are considered to be at the equilibrium position between buccal and lingual forces (62). The covariation in width was expected from epidemiological studies as well. Lack of correlation in the transverse dimension would result in a high percentage of posterior crossbites but the prevalence of posterior crossbite ranges from 2 to less than 20 per cent (63–66) (the prevalence in our orthodontic population sample was expectantly higher). The high covariance in arch width was also reflected in conventional measurements; the upper and lower intermolar distances, as measured between the buccal mesial cusp tips, were significantly correlated ($R^2 = 0.46$, $P < 0.001$). Significant correlations between the transverse dimensions of the upper and lower alveolar processes and dental arches have been reported previously (67, 68).

The second covariation pattern (PLS2) accounted for only 11 per cent of the total covariance and mainly related the maxillary canine vertical position to the mandibular canine labiolingual position. Although no cause and effect relationship can be established, based on the normal dental eruption sequence, this pattern may indicate that a labially positioned mandibular canine could hinder vertical development of the maxillary canine. Contrariwise, lingual positioning of the mandibular canine could allow over eruption of the maxillary canine and result in increased canine overbite.

Concerning the vertical dimension and the steepness of the curve of Spee, we found no appreciable covariation between the two dental arches. In contrast, others have reported a positive correlation between the depths of the curve of Spee in the maxillary and

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**Figure 5.** Plots depicting the sample in form space, showing size difference between males and females, for the upper (a) and lower (b) dental arches. The line represents the vector of pure size change. Blue: males, red: females.
mandibular arch, but their samples included subjects with normal arch shapes and minimal crowding, or normal occlusion (69, 70). It is conceivable that depth of the curve of Spee and overbite are more related to anteroposterior relationship of the arches as a whole, rather than to their individual shape.

The RV coefficient, indicating the total extent of covariation, although statistically significant, was not strong. Approximately two thirds of the shape variation of the arches was independent of each other, thereby allowing a wide range of potential malocclusion configurations. It seems that apart from overall arch shape and width, which may be enforced by intercuspation and muscle equilibrium, different, and relatively independent aetiological factors determine tooth position in each arch. This finding may have clinical implications, indicating that different retention strategies may be appropriate for each arch.

**Limitations**

The main limitations of this research were 1. the sample was taken from an orthodontic setting, thus results may not apply to the general population, 2. age range extended from prepubertal to adult but the sample was cross-sectional and age-related findings must be taken with caution, and 3. the sample was not partitioned based on aetiology of malocclusion.

**Conclusions**

The main shape variation pattern, observed in both arches, was overall arch form, ranging from triangular to square. The other variation patterns were different and characteristic of each arch. Covariation was related to arch width and length and limited to about one-third of the total variance. Integration in the vertical dimension was weak,
mainly restricted to canine position. These results show that each arch displays characteristic patterns of malocclusion that are largely independent between the arches.

References


Figure 8. The main pattern of covariation of the sample. Blue: shape consensus, red: −3SD+3SD configurations.