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Dentistry Section

Original Article

Sizing the Shape: Understanding Morphometrics

NEHA

ABSTRACT

Purpose: One of the most fundamental limitations associated with the conventional cephalometrics is its inability to delineate size from shape as it depends mainly on linear and angular measurements. However, the biological structures warrant greater description in terms of shape and form for better comparison of variation in a particular population. To overcome these shortcomings, morphometrics are now being employed for describing the biological structures in terms of quantifying the shape and form. Also, statistical analysis is being applied to find the variability of this form in the population. The present paper assesses the use of the Procuste superimposition technique and the subsequent form analysis by the principal component analysis (PCA).

Materials and Methods: The lateral cephalograms of 10 adult females were taken from existing records, traced & digitized & then superimposed by means of procuste superimposition. A comparison was made with the conventional superimposition methods based on arbitrary reference planes like cranial base, FHP, SN. The statistical analysis for assessment of shape variability of the structures seen on the lateral cephalogram was done by calculating the principal components for 3 out of these 10 samples.

Results: The conventional superimposition methods do not provide realistic picture of variation in the biological structures as they themselves are prone to variability even in a particular population.

Conclusion: Concepts in Morphometrics can be applied for the purpose of orthodontic assessment of a particular patient with regards to his craniofacial morphology. With the help of morphometrics, norms for a population can be determined based on all the kinds of variations present naturally in that particular population & individuals can thus be compared more realistically regarding the morphological variations.

Keywords: Procustes, PCA (principal component analysis), Statistical shape analysis

INTRODUCTION

Conventional cephalometrics uses linear & angular measurements for the purpose of classification & thus gives a partial & localized description of the differences in the shape of the anatomical structures [1]. Also, structures used as a reference for comparison amongst different individuals are themselves prone to variability and are not biologically constant. Hence, there is a need for a method that better compares two biological entities with regards to variability in their form. Morphometrics is being applied today in all walks of scientific research for analyzing structural characteristics of various organismal forms.

Morphometrics

Morphometrics refers to the quantitative analysis of *form* i.e. it encompasses both size and shape [2]. It is derived from the Greek words "morph", meaning -shape, and "mentron", i.e., measurement, & is used to define size and shape [3]. Morphometric techniques allow the integration of the distinct information present in cephalometry: geometric location and biological homology [4]. Shape was defined by Kendall (1989), "as the information remaining when location, size, and rotational factors are all removed" [5]. Thus, to compare shapes, the non-shape information is removed from the coordinates of landmarks [6].

One method of doing this is:

Procrustes Superimposition

A superimposition method that aims to compare shapes, as defined by landmark configurations, by fitting them with the use of various optimization criteria.

The method involves three steps:

1) Translation (centering of landmark configurations);
2) Rotation (rotation of all landmark configurations to minimize the difference between them);
3) Scaling (size standardization of landmark configuration against the centroid size) [7].

This method translates the centroid of the shapes to (0,0); the *x* coordinate of the centroid is the average of the *x* coordinates of the landmarks of an individual, and the *y* coordinate of the centroid is the average of the *y* coordinates. Shapes are scaled to unit centroid size, which is the square root of the summed squared distances of each landmark to the centroid. Thus the centroid of a shape is composed of landmark points which are the average of all the points (the "center of gravity" of the shape) [8,9]. The configuration is rotated to minimize the deviation between it and a reference, typically the mean shape. Because shape space is curved, analyses are done by projecting shapes onto a space tangent to shape space. Within the tangent space, conventional multivariate statistical methods such as multivariate analysis of variance and multivariate regression, can be used to test statistical hypotheses about shape [10].

Thus the distinguishing feature of geometric morphometrics is that the co-ordinates of the landmarks are statistically analysed, after scaling and alignment, rather than inter- landmark distances. This has the advantage that the results of statistical analyses can be visualized as deformations of landmark configurations and the sensitivity is greater since more shape information is analysed [11].

Types of Procrustes Superimposition:

Partial Procrustes: Translation and rotation without scaling.

Full Procrustes: Translation, rotation, and scaling.

Types of Procrustes Analysis

Ordinary Procrustes Analysis (OPA): Superimposes one landmark configuration on another (reference) configuration.

Generalized Procrustes Analysis (GPA): Takes two or more shapes, finds the average shape, and optimally matches every configuration in the sample to that average.

GPA is a symmetric method (i.e., the order of objects does not matter). OPA is an asymmetric method and its outcome depends on the choice of the reference object [12].

Based on these morphometric methods the anatomical structures can be compared amongst population by finding out the average shape for the population & calculating the amount by which each individual in the population varies or deviates from this average.

Principal Component Analysis

Principal Component Analysis (PCA) was first introduced by Pearson [13] in 1901 and later independently developed by Hotelling [14] in 1933. The other terms used for this analysis are the singular value decomposition (SVD), the Karhunen-Loeve transform, the Hotelling transform, and the empirical orthogonal function (EOF) method.

PCA is a statistical technique for reducing the number of variables when a significant correlation between the variables is present [15]. It is a simple method of extracting relevant information from high dimensional data sets. It is a way of identifying patterns in data, and expressing the data in such a way to highlight their similarities and differences. The position of each point might vary along both the x and y directions; thus there are 2k variables to describe variability, where *k* is the number of points. As the points do not behave independently, because, they all belong to the same biological form; the Principal component analysis decreases the number of variables. Thus it limits the number of variables in the evaluation of biological shapes. However, the components of PCA are arrived at statistically, not from biological considerations.

AIM

The aim of this study was to apply the two principles of:
Procuste superimposition: To elucidate the shortcomings of the conventional superimposition techniques, and

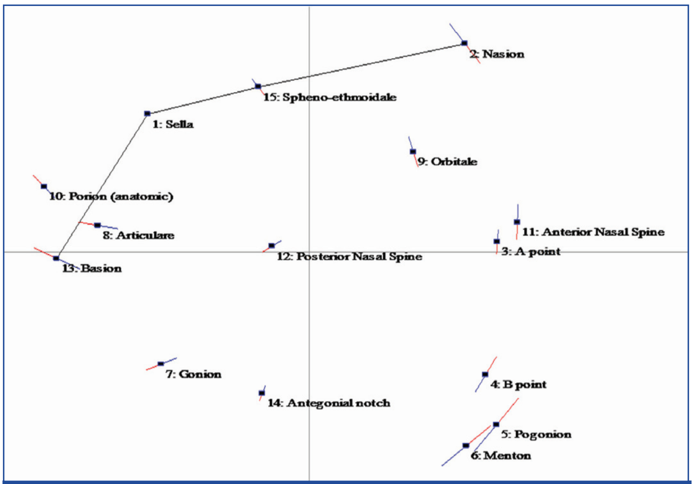
Principal component analysis: To calculate the principal components of a sample based on the sample average.

MATERIALS AND METHODS

The sample consisted of 10 lateral cephalograms of adult females (age range 17-24 years) with a harmonious and orthognathic profile, full complement of teeth, Class I molar relationship with normal overjet and overbite, no history of orthodontic treatment. The radiographs were taken from the existing pre treatment records of patients reporting to the Department of Orthodontics at MCODS, Mangalore for minor orthodontic corrections. The radiographs were traced & then digitized after scanning with the help of Viewbox three software (dHAL software, Kifissia, Greece) .

A set of 15 points was digitized for the purpose of superimposition: [Table/Fig-1] **Points digitized for superimposition**)

1. basion (Ba),
2. sella (S),
3. sphenoethmoidale (Se),
4. nasion (N),
5. porion (Po),
6. orbitale (O),
7. anterior nasal spine (ANS),
8. A point (A),
9. posterior nasal spine (PNS),
10. articulare (Ar),
11. gonion (Go),
12. antegonial notch (Ag),
13. menton (Me),
14. pogonion (Pg),
15. B point (B).



[Table/Fig-1]: Points digitized for superimposition

The tracings were superimposed on this position of best fit & compared with superimposition on conventional reference planes for drawing inferences [16].

For the measurement of shape *Principal Component Analysis* can be applied which was the statistical method used to analyse the average shape and shape variability of the existing sample.

How does PCA compute

Any landmark, for e.g., point A can be described in a two dimensional coordinate with specific value along X & Y axis. Thus, all the cephalometric points under consideration are defined by x & y which forms the data set. This mean configuration of all the forms in the sample under study in terms of average of x and y coordinates is called consensus [17]. The mean shape or the consensus was calculated for three tracings [Table/Fig-2] superimposed by the Procrustes method with respect to 15 previously mentioned points.

i) After the dataset is acquired, the mean is subtracted from the data items.

   This is the average across each dimension. Thus, all the data items in each dimension will have its mean subtracted. This new dataset will thus have a mean whose value is zero.

ii) Covariance matrix is calculated –

   Covariance is a measure of how much two random variables change together. As the data set is 2-dimensional, hence the covariance matrix will be (2x2).

iii) Eigenvectors and eigenvalues of the covariance matrix are calculated: The eigenvectors of a square matrix are the non-zero vectors that, after being multiplied by the matrix, remain parallel to the original vector. For each eigenvector, the corresponding eigenvalue is the factor by which the eigenvector is scaled when multiplied by the matrix. Eigenvectors can be calculated only for square matrices.

This step involves the reduction of dimension. After the eigen vectors are computed, the eigen values are sorted in descending order, giving the principle components in the order of significance [18]. Then, the less significant components can be ignored. Because of this, some of the principal component analysis can be used in morphometric analysis as any point on an anatomical structural will be related to other points on the structure.

The PCs were calculated for the sample and are given in [Table/Fig-3]. Procrustes distance [Table/Fig-4] is calculated as the square root of the sum of squared distances between corresponding points when the shapes are aligned & denotes the difference in shape between two patients that is measured by the distance.

Procrustes residual [Table/Fig-5] is calculated by evaluating the difference between the location of the landmarks of each form (corresponding to each landmark), and the position of the landmark

S. No.	Landmark	X- axis	Y-axis
1.	basion (Ba)	-1.5758481E-001*	-2.2469673E-001
2.	sella (S)	1.9586924E-001	-2.7641150E-001
3.	sphenoethmoidale (Se)	1.9425909E-001	8.1050452E-003
4.	nasion (N)	1.7900437E-001	2.0487204E-001
5.	porion (Po)	1.8716478E-001	2.3300894E-001
6.	orbitale (O)	1.4632724E-001	3.0186048E-001
7.	anterior nasal spine (ANS)	-1.7202674E-001	1.6945815E-001
8.	A point (A)	-2.3198510E-001	-6.1516710E-002
9.	posterior nasal spine (PNS)	1.2757144E-001	-1.4126997E-001
10.	articulare (Ar)	-2.7027317E-001	-1.2182958E-001
11.	gonion (Go)	2.1904195E-001	-1.1579438E-002
12.	antegonial notch (Ag)	-5.0723364E-002	-4.7329933E-003
13.	menton (Me)	-2.6962755E-001	-7.3176399E-003
14.	pogonion (Pg)	-8.1319375E-002	2.1459705E-001
15.	B point (B)	-1.5697992E-002	-2.8254714E-001

[Table/Fig-2]: Consensus (X, Y)
* AE- 00b indicates A x 10^{-b}

	Variance
PC 1:	2.6736683E- 003
PC 2:	9.8449041E- 004
PC 3:	3.3506599E- 006
PC 4:	1.6450244E- 035
PC 5:	1.0015778E- 034
PC 6:	2.7379548E- 038
PC 7:	1.3810797E- 066
PC 8:	3.7675767E- 067
PC 9:	1.6545390E- 069
PC 10:	1.2539649E-097
PC 11:	2.9941989E- 098
PC 12:	2.7478403E- 101
PC 13:	3.0559112E- 130
PC 14:	4.6022564E -130
PC 15:	5.4515983E-133

[Table/Fig-3]: The PCs were calculated for the sample

Sample	Sizes	Procrustes Distances
1	3.1263207E+003	7.0609909E-002
2	3.6221923E+003	4.5682612E-002
3	3.3602748E+003	6.2544925E-002

[Table/Fig-4]: Procustes distances

in the consensus. Thus, we can calculate how each landmark in an individual differs from its average location in the population. These can be plotted to display the shape variance of a configuration [19].

RESULTS

Superimpositions

- Superimposition on the cranial base shows that 2 out of the 10 samples studied have a very steep mandibular plane. The same sample seems to be varied in cranial base angulation when superimposed on the FH plane while the difference in the mandibular plane seen with cranial base superimposition is not that marked.
- Again, superimposition on SN plane shows one subject to be extremely different from the rest of the sample in terms of the mandibular plane angulation & another subject to differ considerably with regards to the palatal plane.

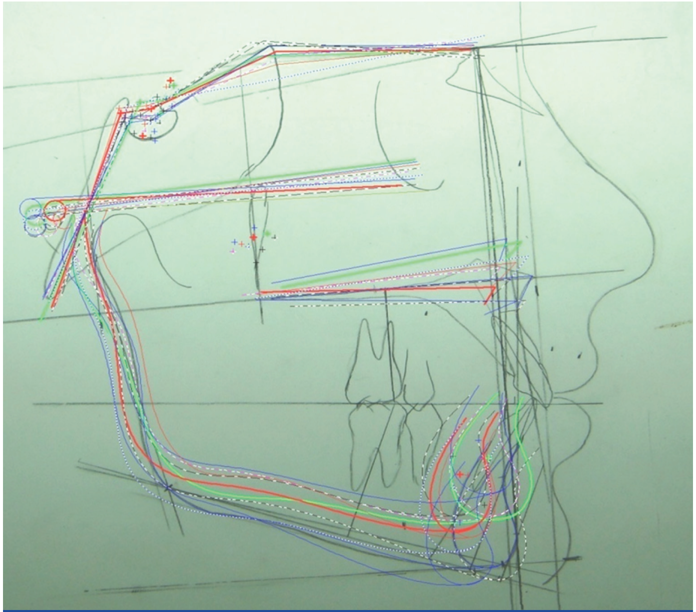
S. No.	Landmark	X	Y
Sample 1			
1.	Ba	1.7133898E-002	6.3747935E-003
2.	S	-1.6475485E-003	-1.2657601E-002
3.	Se	-9.3133775E-003	9.5762138E-003
4.	N	-7.3688091E-003	2.0803880E-002
5.	Po	1.3481543E-002	-5.0053535E-002
6.	O	9.7753982E-003	1.6718260E-002
7.	ANS	-4.7945993E-003	-2.0800465E-003
8.	A	-2.7318457E-003	-1.4078330E-003
9.	PNS	-1.4808971E-003	4.4565421E-003
10.	Ar	-6.0262200E-003	-6.3473722E-003
11.	Go	-1.7898978E-003	1.1348258E-002
12.	Ag	8.5650513E-003	-4.1344565E-003
13.	Me	3.5638658E-003	-9.2264957E-003
14.	Pg	-7.2192641E-003	5.8785870E-003
15.	B	-1.0147297E-002	1.0750806E-002
Sample 2			
1.	Ba	-5.5222486E-003	-9.9076727E-003
2.	S	2.4447871E-003	3.7023053E-005
3.	Se	-1.7429217E-003	-1.6625675E-003
4.	N	-5.7860895E-003	-6.9186744E-003
5.	Po	-1.0824667E-002	1.6508189E-002
6.	O	-1.9475808E-003	-1.0070697E-003
7.	ANS	9.6182492E-003	8.8332808E-003
8.	A	4.1914928E-003	-1.6005052E-002
9.	PNS	2.6223951E-003	7.3582804E-004
10.	Ar	9.3919761E-003	2.9249039E-003
11.	Go	1.9923582E-003	-7.4870854E-003
12.	Ag	-9.6684866E-003	-4.2216302E-004
13.	Me	-1.1300003E-002	1.0998999E-004
14.	Pg	2.1799697E-002	2.8819189E-003
15.	B	-5.2689576E-003	1.1379151E-002
Sample 3			
1.	Ba	-1.0746152E-002	4.7669730E-003
2.	S	-1.8730041E-003	1.4138703E-002
3.	Se	9.9893770E-003	-7.9581614E-003
4.	N	1.2171759E-002	-1.5010417E-002
5.	Po	-3.6848339E-003	3.2265599E-002
6.	O	-8.6314852E-003	-1.7369087E-002
7.	ANS	-3.8788336E-003	-7.6839432E-003
8.	A	-1.8552362E-004	1.7750751E-002
9.	PNS	-1.8421540E-003	-4.4164781E-003
10.	Ar	-1.8813445E-003	4.0915885E-003
11.	Go	-1.4054966E-003	-3.7975751E-003
12.	Ag	1.3820215E-003	4.5826143E-003
13.	Me	9.2170032E-003	9.1566962E-003
14.	Pg	-1.4133806E-002	-9.9391296E-003
15.	B	1.5502472E-002	-2.0578134E-002

[Table/Fig-5]: Residuals (X, Y)

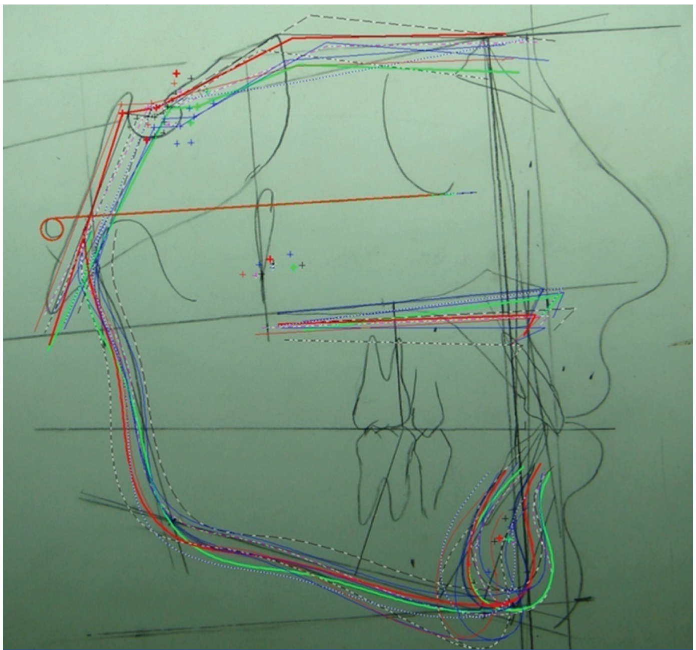
- On the other hand, superimposition according to the procuste principles demonstrates a continuum of variation as it is based on the whole of the population & not on any arbitrary plane which itself is prone to variations.

  Sum of Procrustes distances: 1.7883745E-001

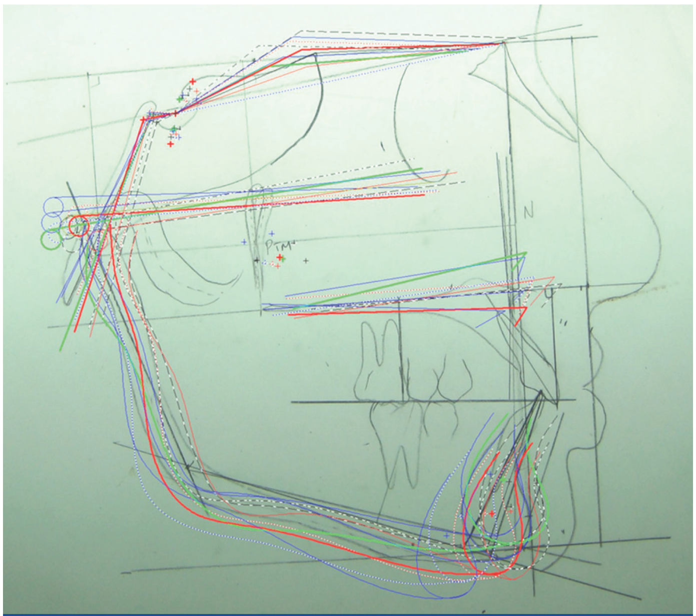
  Sum of Squared Procrustes distances: 1.0984528E-002



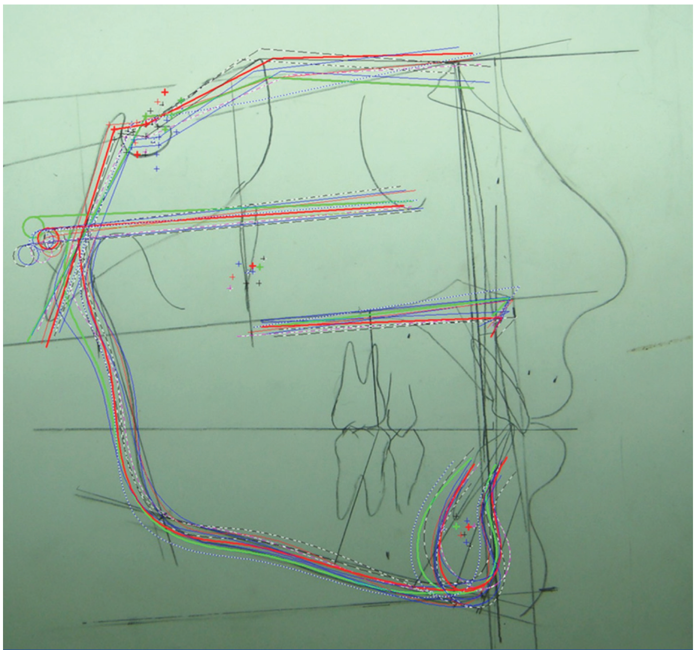
[Table/Fig-6]: Superimposition on cranial base



[Table/Fig-7]: Superimposition on FH plane



[Table/Fig-8]: Superimposition on SN plane



[Table/Fig-9]: Superimposition on Procuste

DISCUSSION

Superimposition: The results of superimposition demonstrate that the choice of reference plane has a great bearing on the variations in the sample that emerge out of such a comparison [Table/Fig-1,6-9]. It is only the Procustes superimposition which is based on the average of population that best describes the deviation of the structural form of a particular subject in the population. The other planes of references may themselves vary and thus changing the plane of reference changes the interpretation of the outcome of superimposition. This has also been demonstrated by Halazonetis wherein he has superimposed two tracings on arbitrary orientation, SN plane and by Procustes method [9].

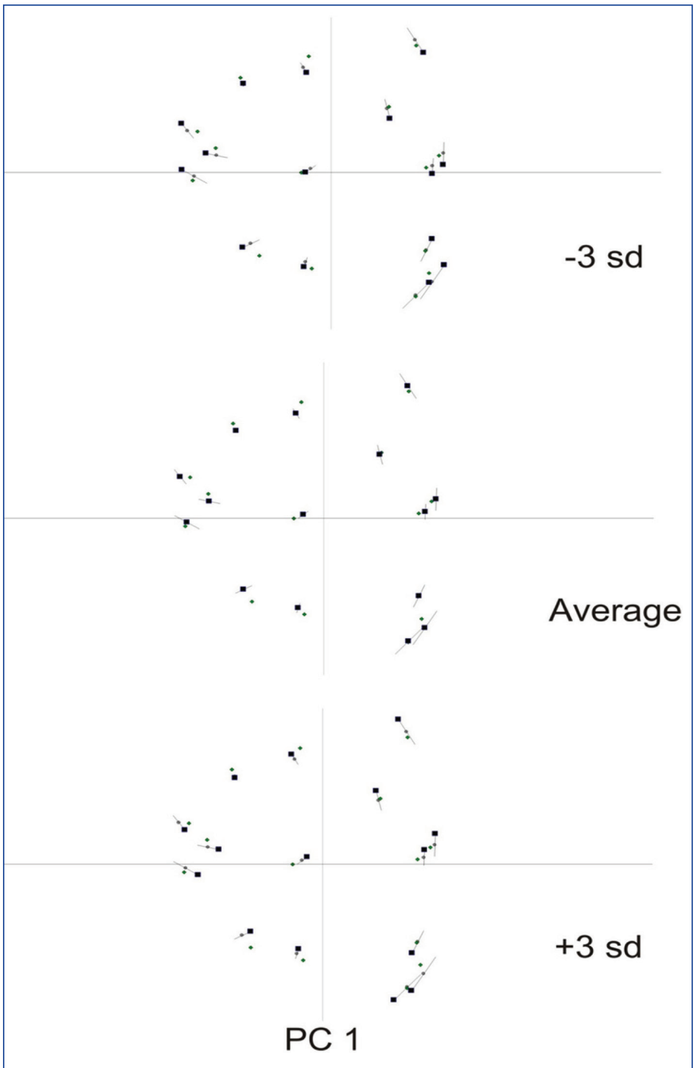
PCA: The PCs place the patient at the appropriate position in the population's shape-space. The first PCs describe the shape pattern in general terms, and successive PCs concentrate on finer detail. For broad classification, 2 or 3 PCs might be sufficient. Here, the first 2 PCs are shown & the Average shape (middle) was warped by applying each PC by amount equal to 3 standard deviations in negative (left) and positive (right) direction {[Table/Fig-10]: PC1 with standard deviation, [Table/Fig-11] PC 2 with standard deviation}.

Shape between patients can be compared by the Procrustes distance. This might be particularly helpful when planning the treatment of a new patient, because it allows retrieval of data for previously treated patients of a similar pattern to consider their responses to treatment uniformly scale their experimental groups as a precursor to further morphometric analyses.

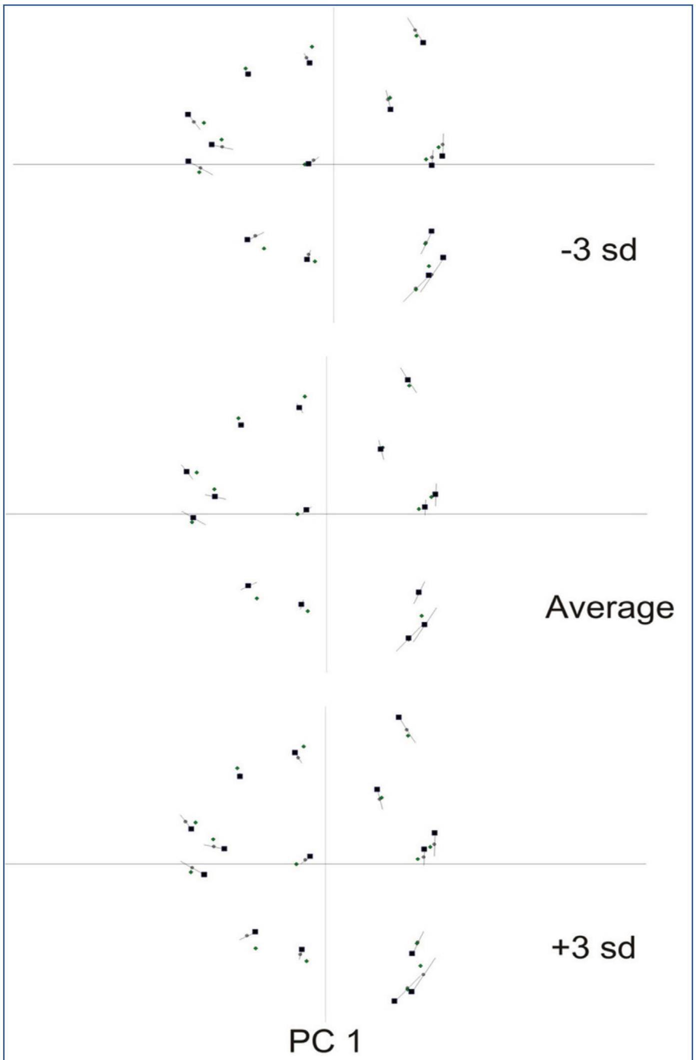
The procustes analysis has been used in various studies for bringing out variation in craniofacial form in the field of orthodontics. Henessey and Moss analysed change in facial shape independently of change in size with age by calculating the Principal Components based on 22 facial landmarks [11]. They found that PC-1 showed significant correlation in shape change versus age amounting to 40% of total variance for each subject.

Facial variation was also assesed by Toma et al., in 4747 British school children by calculating 14 PCs explaining 82% of total variance with the first 3 components accounting for 46% variance [20].

In a study by Wellens, Procustes analysis was used to fit the 12-year male- female averaged Bolton template on the patient's digitized landmarks and to combine the template's reference landmarks/ planes with the patient's points A and B to determine the normalized



[Table/Fig-10]: PC1 with standard deviation



[Table/Fig-11]: PC 2 with standard deviation

measurements for determining sagittal discrepancy [21]. They reported increase in the correlation between the various analyses in comparison with their classic counterparts through the use of geometric morphometrics.

Morphometrics has also been used to assess the treatment outcome in orthodontics. Nogueira et al., have evaluated the morphometric changes of condylar cartilage in growing rats in response to mandibular retractive forces and found significant changes with respect to each layer of the cartilage [22].

Mc Intyre and Mossey have evaluated the advantages and limitations of the geometric morphometric methods currently used to analyse the craniofacial morphology on cephalograms like CCA, Procrustes superimposition, Euclidean distance matrix analysis (EDMA), thin-plate spline analysis (TPS), finite element morphometry (FEM), elliptical Fourier functions (EFF), and medial axis analysis (MAA) [23].

The present study illustrates the use of morphometrics in the field of Orthodontics and the investigated the method of its application for a given sample for the purpose of comparison of craniofacial form. This information forms an essential part of the Orthodontic armamentarium for proper assesment, diagnosis and hence the treatment planning.

CONCLUSION

The choice of reference plane for superimposition greatly affects the inferences that can be derived while studying the variations in the form of biological structures in the population.

The assessment based on all the kinds of variations present naturally in the particular population & not on few rigid criteria of ideal characteristics would be and would encompasse a greater number of parameters.

Thus, concepts in Morphometrics can be applied for the purpose of orthodontic assessment of a particular patient with regards to his craniofacial morphology giving a more complete and realistic comparison.

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