A Bioinformatics Approach to 3D Shape Matching

Manuele Bicego(✉), Stefano Danese, Simone Melzi, and Umberto Castellani

Dipartimento di Informatica, University of Verona,
Strada le Grazie 15, 37134 Verona, Italy
manuele.bicego@univr.it

Abstract. In this paper we exploit the effectiveness of bioinformatics tools to deal with 3D shape matching. The key idea is to transform the shape into a biological sequence and take advantage of bioinformatics tools for sequence alignment to improve shape matching. In order to extract a reliable ordering of mesh vertices we employ the spectral-based sequencing method derived from the well known *Fiedler Vector*. Local geometric features are then collected and quantized into a finite set of discrete values in analogy with *nucleotide* or *aminoacid* sequence. Two standard biological sequence matching strategies are employed aiming at evaluating both local and global alignment methods. Preliminary experiments are performed on standard non-rigid shape datasets by showing promising results in comparison with other methods.

Keywords: Non-rigid shape matching · Biological sequence alignment · Spectral mesh processing · Local geometry

1 Introduction

The research in Computational Biology and Bioinformatics experienced an unprecedented growth in recent years, tying together many disciplines and fields of computer science. In particular, very often Pattern Recognition/Machine Learning techniques are used to solve problems and extract knowledge from biological data [2]. There are lots of motivations for exploiting these disciplines: it is possible to "learn from examples", derive quantitative models, handle non vectorial data, and deal with many classification, clustering and detection problems commonly encountered in the life sciences. In many cases, Pattern Recognition techniques can not be applied "as they are"; researchers spent large efforts to tailor and adapt techniques, so that biological constraints and needs are taken into account. Sometimes, this led very far away from the original methodology, with a clear example in the profile-HMMs [10].

Provocatively speaking, this tight interaction is mainly unidirectional, with the biology/life science side earning the largest benefit. Very recently, an alternative way of interaction has started to be investigated [3,6,21,22]: translate advanced bioinformatics solutions into ideas and methodologies useful to solve

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a pattern recognition problem. The main goal in such contexts is to answer to the following intriguing question: *can we reverse the way of interaction?*, or, in other words, *can we exploit advanced bioinformatics models and solutions to solve pattern recognition tasks?* This perspective is rather new in the literature, with only few relevant examples [3,6,21,22]: in particular, in the video genome project[1] [6], aimed at analysing video sequences, authors established an analogy between biological sequences and videos: in particular, the authors defined the so called "video-DNA", a way to map features extracted from video frames into nucleotidic biological sequences: given the analogy, many different video analysis problems can be faced using the huge range of effective, optimised, and interpretable bioinformatics tools derived from more than 40 years of research. For example authors were able to search for videos using the famous BLAST [1] – a surprisingly fast and effective heuristic-driven algorithm for biological sequence retrieval. In [3,21,22], authors exploited the analogies which can be established between the contour of a 2D shape and a biological sequence to face the 2D shape classification problem with biological sequence alignment tools. They show in [3,22] that, even if employing very basic matching techniques, really promising results can be obtained on different datasets. Moreover, in [21] authors demonstrated that a careful and context-aware setting of the parameters of the biological sequence alignment tools permit to improve even more the obtained accuracies.

This paper is inserted in the above-described context, and explores the possibility of exploiting bioinformatics solutions to face the 3D shape matching problem. Matching of 3D shapes represents an important field in Pattern Recognition and Computer vision research, with various efficient approaches (see [7,14,17,20] for recent surveyes). In general ideal shape matching methods should be highly discriminative and invariant to pose and shape deformations [27]. The majority of methods are focused on effective shape representation aiming at compactly characterizing the shape by a *signature* (or shape *descriptor* [12,20,30]). A large class of methods are based on the matching between the whole shapes by defining a *global* shape descriptor [12,27,30]. Conversely, many approaches are exploiting *local* signatures by leading to a point-to-point matching [8,28]. Recently a lot of work has been proposed to combine *local* and *global* methods by extending the so called *Bag of Words* paradigm to 3D shapes [5,31].

In this paper rather than focusing on the kind of descriptor we propose to pay more attention on the matching phase by facing the 3D shape matching problem with biological sequence analysis tools. The key idea consists of encoding the 3D shape as a biological sequence and employing tailored bioinformatics tools to perform the matching. In order to extract the biological sequence from a 3D shape we exploit spectral-based mesh sequencing methods. As proposed for streaming mesh [13] or mesh partitioning [18] we used the order provided by the second eigenvector of the Laplace operator, usually referred to as *Fiedler Vector*. Then, we collect the shape index [16] at each vertex of the shape as local geometric feature. The ordered sequence of local geometry features is then mapped

[1] See http://v-nome.org/about.html

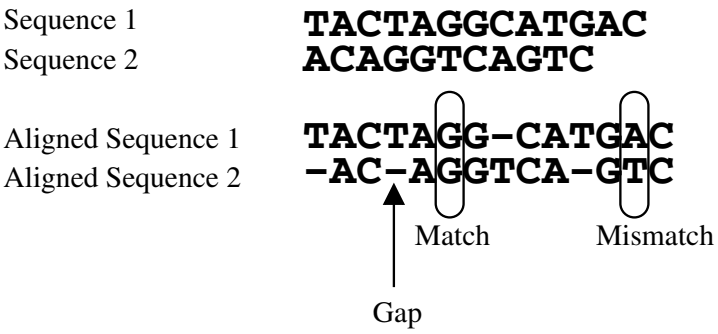

Fig. 1. Alignment of two sequences

into a biological sequence with two simple mappings, one leading to a nucleotide sequence, the other leading to an aminoacid sequence. Once encoded 3D shapes in biological sequences, we employed standard sequence alignment tools (like the Smith-Waterman [29] and the Needleman-Wunch [24] algorithms) to devise a sequence similarity measure. Such similarity is finally used in a standard nearest neighbour classification scenario. Moreover, the alignment procedure provides us a robust estimation of corresponding points among shape pairs.

We tested our approach in matching non-rigid shapes with strong pose variations from two standard datasets: Tosca [4] and Shape Google [5]. Even if we applied a very simple mapping as well as the basic standard bioinformatics solutions to this problem, we obtained very promising results, also in comparison with the state of the art.

2 Background: Biological Sequence Alignment

Analysis of biological sequences is of paramount importance in biology and medicine, very often representing the basic operation in many computational biology and bioinformatics analyses. Broadly speaking, biological sequences are of two types: nucleotide sequences – i.e. strings made with the 4 symbols of DNA, namely $ATCG$ – and aminoacid sequences – i.e. strings with symbols coming from a 20 letters alphabet. Intuitively, the alignment of two sequences is aimed at finding the best registration between them (namely the best way of superimposing one sequence on the other). From a practical point of view, alignment is obtained by inserting spaces inside the sequences (the so called *gaps*) in order to maximize the point to point similarity between them – see Fig. 1. A huge amount of approaches have been proposed in the past to face this problem (see [15,19] for recent reviews and perspectives on the topic), with already effective methods aged in the seventies or early eighties [24,29]. Broadly, we can classify them into pairwise and multiple alignment approaches, with the former devoted at finding the best registration of two sequences and the latter

aimed ad finding a simultaneous alignment of more than two sequences. Another interesting classification is among global or local alignment approaches: global methods try to find the best overall alignment between sequences, whereas the local alignment aims at finding short regions of highly similar sequences. A thorough treatment of this topic is of course out of the scope of this paper. Here, since we are interested in investigating the basic potentialities of our ideas, we chose two very basic pairwise alignment tools (namely the Needleman-Wunsch [24] and the Smith-Waterman [29] algorithms), representing the reference in this field – being extensively employed since their proposal in the seventies/eighties.

In particular, the NeedlemanWunsch algorithm [24] is a dynamic programming method for finding the best *global* alignment between two sequences – it represents the first application of dynamic programming to biological sequence comparison. The basic idea is to maximize the similarity between two sequences by *i)* making use of a similarity matrix (also called Scoring Matrix) which defines the similarity between every pair of symbols in the alphabet and *ii)* by taking into account penalty values for gap opening and extension. There are many possible scoring matrices, which are typically built on the basis of biological knowledge[2].

On the other side, the Smith-Waterman algorithm [29] is a dynamic programming method for local alignment, which identifies homologous regions (i.e., roughly speaking, similar regions) between sequences by searching for optimal local alignments. Instead of looking at an entire sequence at once, the S-W algorithm compares multi-lengthed segments, looking for whichever segment maximizes the scoring measure. A scoring system is used, which includes a set of specified gap penalties.

3 The Proposed Method

The main steps of our proposed pipeline are i) spectral-based shape sequencing, ii) local feature extraction, iii) mapping into biological sequences, and iv) shape matching by sequence alignment. Figure 2 shows the scheme of proposed method. In order to highlight the effectiveness of proposed pipeline we show in Figure 3 the geometric processing of two shapes of the same class in two different poses (i.e., strong isometric transformation). It is interesting to observe that Fiedler vector defines a vertex ordering that goes from the tip of the tail to the head of the cat for both the shapes. Moreover, the extracted local geometric features, namely the Shape index, highlights coherently the semantic components of the cat (see for example the eyes, the ears, and the paws). In the following we introduce more theoretical details of the proposed approach.

3.1 Spectral-Based Shape Sequencing

Let $\mathcal{M}$ be a mesh with N-vertices. A function on $\mathcal{M}$ has a discrete representation specified by a vector with N components. A Mesh Laplacian is a linear operator

[2] For example, in the nucleotide case, it is known from the chemical composition of DNA basis that it is more difficult to have a change from an Adedine to a Thymine rather than to a Guanine.

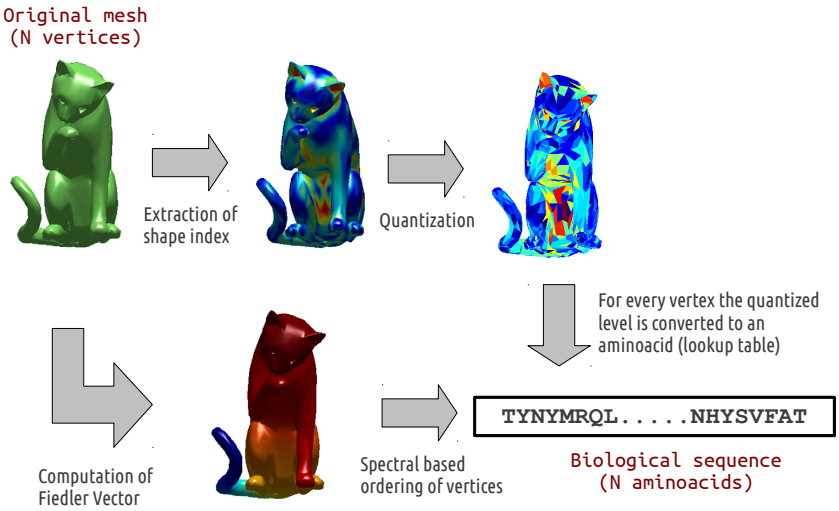

Fig. 2. Scheme of proposed method

L defined by a $N \times N$ matrix [32]:

$$(L\mathbf{f})_i = b_i^{-1} \sum_{j \in N(i)} w_{ij}(f_i - f_j), \tag{1}$$

and it can be factored into the product of a diagonal and a symmetric matrix

$$L = B^{-1}S, \tag{2}$$

where B^{-1} is a diagonal matrix whose diagonal entries are b_i^{-1} and S is a symmetric matrix whose diagonal entries are given by $s_{ii} = \sum_{j \in N(i)} w_{ij}$ and whose off diagonal entries are $-w_{ij}$. A particular class of mesh Laplacians is defined by the discrete Laplace-Beltrami operator for Riemannian manifold. Here, we use the so called *cotangent* weighting scheme [23,26]. It is well known that from the Laplace Beltrami mesh operator it is possible to obtain an ordering of its vertices. Consider the problem of embedding vertices in the line. This problem is mathematically equivalent to seek a permutation $\pi : V \longrightarrow \{1,\ 2,\ ...,\ n\}$ of the vertices of a mesh $\mathcal{M} = (V, E)$. A solution to this problem can be given by the so called *Fiedler Vector* [11], i.e., the eigenvector associated with the smallest non-zero eigenvalue of L. In other words, the Fiedler vector provides a way to order the vertices of the mesh: by following this order we can derive a sequence of vertices, to be characterized via local geometric properties (i.e., shape index) and translated into biological symbols.

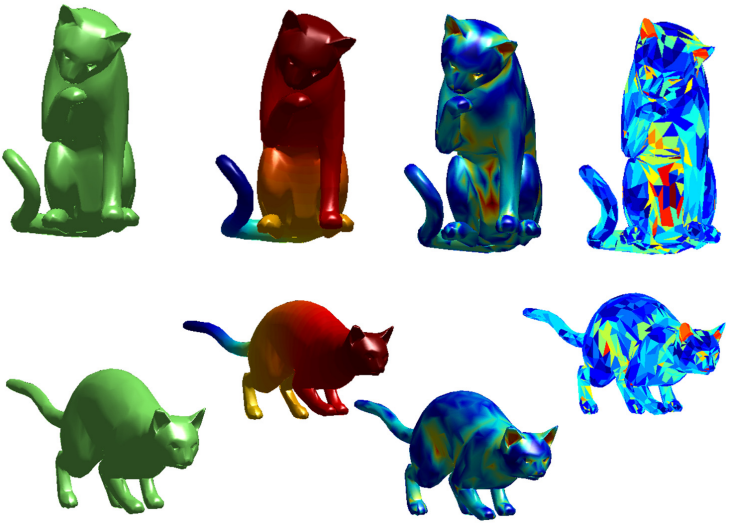

Fig. 3. Geometric processing of two isometric shapes. From left to right: original shapes, Fiedler vector, Shape Index, and shape quantization.

3.2 Local Feature Extraction

We encode local geometric properties of the surface using the *Shape Index* [16], which is defined as:

$$si = -\frac{2}{\pi} \arctan\left(\frac{k_1 + k_2}{k_1 - k_2}\right) \quad k_1 > k_2,$$

where k_1, k_2 are the principal curvatures of a generic vertex. The Shape Index varies in $[-1, 1]$ and provides a local categorization of the shape into primitive forms such as spherical cap and cup, rut, ridge, trough, or saddle [16]. Shape index is scale invariant [16] and it has already been successfully employed for surface matching [8].

3.3 Mapping Into Biological Sequences

Once obtained from the mesh, the ordered sequence of shape indeces should be converted into a biological sequence, in order to permit the mapping. It is interesting to note that there is a strict parallelism between this sequence-based encoding of 3D surfaces and the protein: in both cases the matching is based on the sequences, which are determining the 3D shape (proteins are sequences of aminoacids folded in 3D).

Even if different schemes for mapping shape indeces to aminoacids can be adopted, here we investigated two very simple schemes, both having pros and cons:

- *DNA-mapping*: in this case the shape index is directly mapped to the ATCG alphabet of DNA sequences. We divided the [-1:1] interval into 3 zones ([-1:-0.3], (-0.3:0.3), [0.3 1]), which roughly correspond to values indicating concavity, convexity and saddle characteristics of the surface. Then, each zone is mapped to a different nucleotide (with one character left out), thus transforming the 3D shape into a sequence of highly identifiable geometric characteristics, which are directly mapped into nucleotides. The disadvantage of this encoding scheme is that the quantization is rather heavy (only three symbols), this possibly leading to a loss of details.
- *Protein-mapping*: this method tries to overcome the problems of the previous scheme by exploiting the aminoacid alphabet, which is composed by 20 symbols. Againg we split the shape index range into 20 equally spaced intervals, each one corresponding to an aminoacid. In this way the loss of details derived from the quantization may be less crucial; on the other side, the geometric interpretation can be partially lost.

3.4 Shape Matching by Sequence Alignment

Given the encoding, the alignment of the two obtained biological sequences straightforwardly permits to define a classification strategy based on standard Nearest Neighbour (NN) classifier [9]. We are aware that, given a similarity matrix, interesting alternatives to NN exist (e.g. the dissimilarity-based representation paradigm [25]). However, NN remains rather accurate, still being enough simple to demonstrate the suitability of our proposed approach. Note that in this paper we are more interested in showing the feasibility of our perspective, rather than reaching state of the art results. Moreover, this technique is really interpretable, since it gives an intuitive motivation of the assigned class label by showing the nearest neighbour to the user. In more detail, NN classifier, given an unknown object X and a distance, finds the point in the training set which is nearest to X, assigning X to the class of that point. This is a natural choice, since given our framework it is straightforward to define a distance between 2D shapes: after encoding the two 3D shapes into biological sequences, we can align them and use the alignment error as a measure of distance.

In our experiments we used both local and global alignment tools: in particular, again for being as basic as possible, we employed the two historical approaches described in previous section, namely the Needleman-Wunsch [24] and the Smith-Waterman [29] algorithms. Moreover, we normalize the alignment score by the averaged length of the two involved sequences.

4 Experiments

We evaluated the proposed approach on two 3D shape matching scenarios. We exploited the following variants of the matching algorithm:

- SW / NW: the two alignment algorithms used: SW stands for Smith-Waterman, NW for Needleman-Wunch

- AA / NT: the two coding strategies employed: AA represents the protein coding (i.e. using 20 aminoacids), NT represents the DNA coding (i.e. using the four nucleotides)
- Basic / Advanced: this option refers to the alignment parameters. Actually two are the parameters that should be defined when aligning two biological sequences: the scoring matrix and the gap opening/extending penalty. As explained in the previous Sections, the former defines the price of every substitution in the matrix, whereas the latter defines the penalty in the similarity got while opening (or extending) a gap region. These two parameters typically have a clear biological meaning, and can change drastically the final result. In this preliminary evaluation, we performed two sets of experiments: in the former (referred to as "Basic") we tried to keep as easiest as possible the scheme, leaving such parameters as set by default in the Matlab implementation (Matlab bioinformatics toolbox); in the latter (referred to as "Advanced") we relaxed one biological assumption which does not hold in the shape classification case – this being of course only the first step through the tailoring of the sequence alignment tools to our problem. In particular we observe that in biology the gap penalty is typically high: it is not really desirable to break a biological sequence. In the shape case, nevertheless, such a strong constraint does not hold: actually, gaps can really help in dealing with occlusions and – mainly – scale changes.

We compared the best results of our approach with the following methods:

- Shape DNA method [27] as gold standard for non-rigid shape matching.
- DTW: Dynamic Time warping distance between the Shape Index sequences ordered with the Fiedler Vector. We used a 10% warping window constraint, which is the customary setting in the speech recognition community.
- Histogram of Shape Index as basic shape descriptor. We considered 20, 50, 100, 150, 200, 300 bins, reporting in the table only the best result.

In our first experiment we employed the Tosca *non-rigid world* dataset [4] composed of 10 classes of non-rigid objects: cat, centaur, man1, dog, gorilla, man2, horse, lioness, seahorse, and woman (see Figure 4). For each class there are different number of samples by leading to a total of 143 models. Table 1 reports classification errors obtained using the Leave One Out (LOO) protocol. Our approach reaches the best classification score with several sequence matching approaches by outperforming in particular Shape DNA method. DTW performed better than simple Shape Index histogram by confirming the reliability of the ordering extracted from the Fiedler vector.

As mentioned before, the advantage of the proposed biologically inspired method consists of performing a robust alignment of the input sequences that leads in our case to the estimation of an (incomplete) point-to-point matching. In order to visually evaluate this procedure we plotted the estimated matching among some pairs of shapes from Tosca dataset. Figure 5 shows the estimated correspondences where only fully matched pairs of points are highlighted. It is interesting to observe that correspondences are quite convincing. For instance

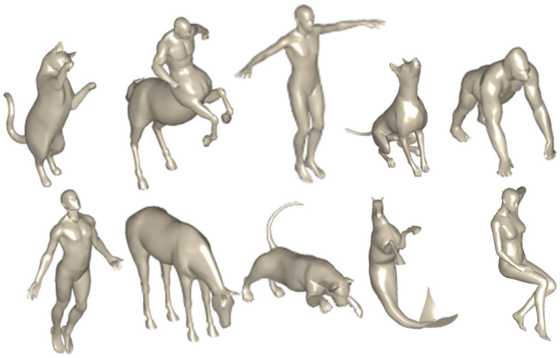

Fig. 4. Tosca non-rigid objects: cat, centaur, man1, dog, gorilla, man2, horse, lioness, seahorse, and woman

Table 1. Results with Tosca dataset

Method	AA	NT
NW (Basic)	**0.0000**	0.0350
SW (Basic)	0.0629	0.1189
NW (Advanced)	**0.0000**	0.1888
SW (Advanced)	0.0629	0.2308

Method	Error LOO
Shape DNA	0.0070
Shape Index Hist (100 bin)	0.0839
DTW	0.0420
Proposed approach (best)	**0.0000**

the paws of the cats or the heads of the horses are correctly matching. Note that due to the symmetry of the shapes some correspondences are switched from left to right side (see for example the fingers or right and left hands of man pair). Finally, it is worth noting that the alignment fails in presence of strong shape partiality like in the case of matching between man and centaur (see Figure 5 bottom right). Clearly this aspect has to be investigated more thoroughly in our future research, as done for example in the 2D shape classification case in [21].

The second experiment is evaluated on a subset of the Shape Google dataset [5]. The dataset is composed of 10 classes of non-rigid objects: dog, cat1, cat2, woman, man, dromedary, elephant, flamingo, horse, cougar. Each object appeared with multiple modifications and transformations of the original shape. Here we evaluated isometry and isometry-topology transformations with five different strength levels (see isometry-topology transformations in Figure 6).

Tables 2 and 3 show classification results. Our approach showed the best results also in this case by confirming the robustness of the proposed methods

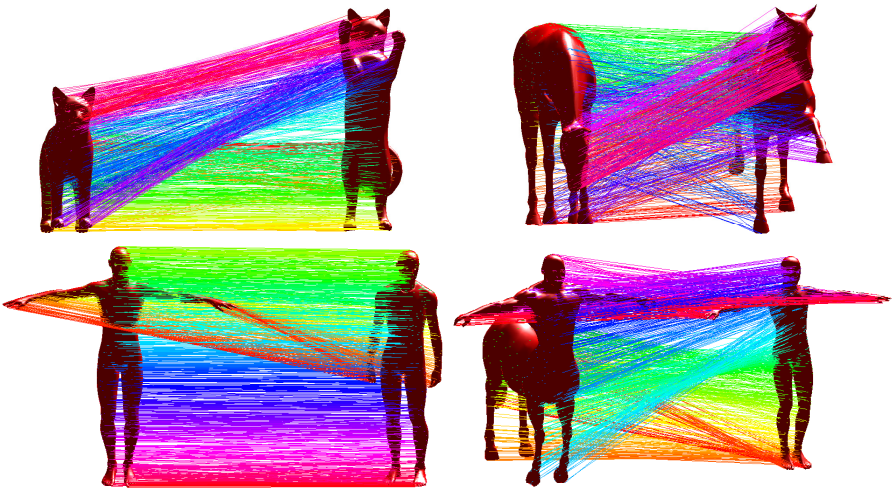

Fig. 5. Point to point matching

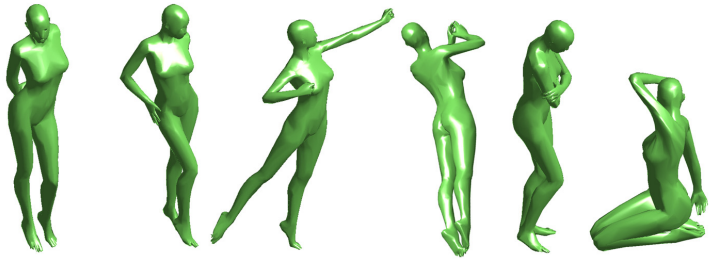

Fig. 6. ShapeGoogle dataset: null shape (left) and five different strength levels of topological and isometric transformation

against strong shape deformations. In particular, zero error is observed for several configurations. Here, it seems evident that errors introduced by topological noise are compensated by the robustness of the biological sequence matching algorithms.

As a final observation, let us try to understand the behaviour of the different variants of the proposed approach. Concerning the alignment algorithm, it seems that the global method (NW) performs better than the local one (SW): actually local methods can be more useful when trying to match objects with occlusions, not present in the analysed dataset. Concerning the encoding methods, the AA version seems to be more adequate, especially in the ShapeGoogle dataset: probably the quantization derived from the NT scheme is too strong in this case, destroying information which is useful for matching.

Table 2. Results with ShapeGoogle-isometry dataset

Method	AA	NT
NW (Basic)	0.0408	0.1224
SW (Basic)	0.0612	0.1429
NW (Advanced)	**0.0000**	0.1020
SW (Advanced)	**0.0000**	0.1020

Method	Error LOO
Shape DNA	0.1020
Shape Index Hist (20 bin)	0.1837
DTW	0.0408
Proposed approach (best)	**0.0000**

Table 3. Results with ShapeGoogle-isometry-topology dataset

Method	AA	NT
NW (Basic)	**0.0000**	0.1837
SW (Basic)	**0.0000**	0.2245
NW (Advanced)	**0.0000**	0.1224
SW (Advanced)	**0.0000**	0.1224

Method	Error LOO
Shape DNA	0.3469
Shape Index Hist (20 bin)	0.2041
DTW	0.1224
Proposed approach (best)	**0.0000**

5 Conclusions

In this paper we focus on the matching phase in non-rigid 3D shape comparison problems. We show how bioinformatics methods can be useful to cope with shape alignment by encoding a 3D mesh as a discrete biological sequence. A well defined pipeline is introduced to address the problems of vertex sequences, local shape description and quantization, and shape classification by sequence alignment. Despite the fact that each single step is simple and well known, the overall method has shown promising results and encourages us to further exploit the idea of 3D matching approaches with established bioinformatics tools. Once a correspondence between 3D shapes and biological sequences is defined, many other interesting information can be extracted (to detect interesting parts, or to do mesh segmentation), by exploiting the huge amount of bioinformatics tools developed in more than 40 years of research.

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