

LB_Keogh Supports Exact Indexing of Shapes under Rotation Invariance with Arbitrary Representations and Distance Measures

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Dear Reader: This is an expanded version of our VLDB paper

Abstract Shape matching and indexing is important topic in its own right, and is a fundamental subroutine in most shape data mining algorithms. Given the ubiquity of shape, shape matching is an important problem with applications in domains as diverse as biometrics, industry, medicine, zoology and anthropology. The distance/similarity measure for used for shape matching must be invariant to many distortions, including scale, offset, noise, articulation, partial occlusion, etc. Most of these distortions are relatively easy to handle, either in the representation of the data or in the similarity measure used. However rotation invariance is noted in the literature as being an especially difficult challenge. Current approaches typically try to achieve rotation invariance in the representation of the data, at the expense of discrimination ability, or in the distance measure, at the expense of efficiency. In this work we show that we can take the slow but accurate approaches and dramatically speed them up. On real world problems our technique can take current approaches and make them four orders of magnitude faster, without false dismissals. Moreover, our technique can be used with any of the dozens of existing shape representations and with all the most popular distance measures including Euclidean distance, Dynamic Time Warping and Longest Common Subsequence. We further show that our indexing technique can be used to index star light curves, an important type of astronomical data, without modification.

Keywords Shape, Indexing, Dynamic Time Warping

1. INTRODUCTION

Shape matching and indexing is important topic in its own right, and is a fundamental subroutine in most shape data mining algorithms. Given the ubiquity of shape, shape matching is an important problem with applications in domains as diverse as biometrics, industry, medicine, zoology and anthropology. The

distance/similarity measure for used for shape matching must be invariant to many distortions, including scale, offset, noise, articulation, partial occlusion, etc.. Figure 1 gives a visual intuition of these problems in a familiar domain, butterflies and moths. Most of these distortions are relatively easy to handle, particularly if we use the well-known technique of converting the shapes into time series as in Figure 2. However, no matter what representation is used, rotation invariance seems to be uniquely difficult to handle. For example [20] notes “rotation is always something hard to handle compared with translation and scaling”.

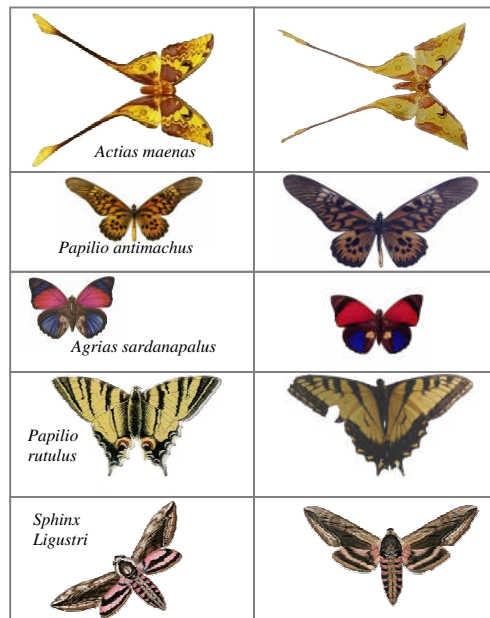


Figure 1: Examples of the distortions we may be interested in being invariant to when matching shapes. The left column shows drawings of insects dating back to 1734 [32]. The right column shows real insects. The flexible wingtips of *Actias maenas* require articulation invariance. One of the *Papilio antimachus* must be resized before matching. The *Agrias sardanapalus* need their offsets corrected in order to match. The real *Papilio rutulus* has a broken wing which appears as an occlusion to shape matching algorithms. The real *Sphinx Ligustri* needs to be rotated to match the drawing, achieving this invariance is the focus of this work

Many current approaches try to achieve rotation invariance in the representation of the data, at the expense of discrimination ability [28], or in the distance measure, at the expense of efficiency [1][2][3][9].

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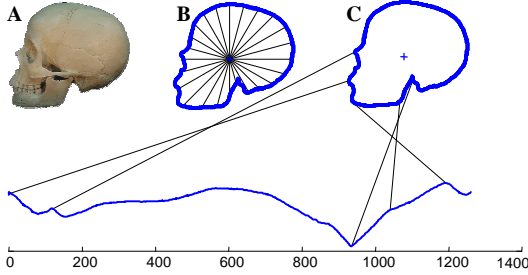


Figure 2: Shapes can be converted to time series. **A)** A bitmap of a human skull. **B)** The distance from every point on the profile to the center is measured and treated as the Y-axis of a time series of length n (**C)**

As an example of the former, the very efficient rotation invariant technique of [28] cannot differentiate between the shapes of the lowercase letters “d” and “b”. As an example of the latter, the work of Adamek and Connor [1], which is state of the art in terms of accuracy or precision/recall takes an untenable $O(n^3)$ for each shape comparison.

In this work we show that we can take the slow but accurate approaches and dramatically speed them up. For example we can take the $O(n^3)$ approach of [1] and on real world problems bring the average complexity down to $O(n^{1.06})$. This dramatic improvement in efficiency does not come at the expense of accuracy; we prove that we will always return the same answer set as the slower methods.

We achieve speedup over the existing methods in two ways, dramatically decreasing the CPU requirements, and allowing indexing. Our technique works by grouping together similar rotations, and defining an admissible lower bound to that group. Given such a lower bound, we can utilize the many search and indexing techniques known in the database community.

Our technique has the following advantages:

- There are dozens of techniques in the literature for converting shapes to time series [1][3][7][38][39][44], including some that are domain specific [5][31]. Our approach works for *any* of these representations.
- While there are many distance measures for shapes in the literature, Euclidean distance, Dynamic Time Warping [2][5] [30][31] and Longest Common Subsequence [37] accounts for the majority of the literature. Our approach works for *any* of these distance measures.
- Our approach uses the idea of LB_Keogh lower bounding as its cornerstone. Since the introduction of this idea a few years ago [16], dozens of researchers world wide have adopted and extended this framework for applications as diverse as motion capture indexing [18], P2P searching [13], handwriting retrieval [31], dance indexing, and query by humming and monitoring streams [40]. This widespread adoption of LB_Keogh lower bounding has insured that it has become a mature and widely supported technology, and suggests that any contributions made here can be rapidly adopted and expanded.
- In some domains it may be useful to express *rotation-limited* queries. For example, in order to robustly retrieve examples of the number “8”, without retrieving infinity symbols “∞”, we can issue a query such as: “Find the best match to this shape allowing a maximum rotation of ± 15 degrees”. Our framework supports such rotation-limited queries.

The rest of this paper is organized as follows. In Section 2 we discuss background material and related work. In Section 3 we formally introduce the problem and in Section 4 we offer our solution. Section 5 offers a comprehensive empirical evaluation of both the effectiveness and efficiency of our technique. Finally Section 6 offers some conclusions and directions for future work.

2. BACKGROUND AND RELATED WORK

The literature on shape matching is vast; we refer the interested reader to [7][36] and [44] for excellent surveys. While not all work on shape matching uses a 1D representation of the 2D shapes, an increasingly large majority of the literature does. We therefore only consider such approaches here. Note that we lose little by this omission. The two most popular measures that operate directly in the image space, the Chamfer [6] and Hausdorff [27] distance measures, require $O(n^2 \log n)$ time¹ and recent experiments (including some in this work) suggest that 1D representations can achieve comparable or superior accuracy.

In essence there are three major techniques for dealing with rotation invariance, landmarking, rotation invariant features and brute force rotation alignment. We consider each below.

2.1 Landmarking

The idea of “landmarking” is to find the one “true” rotation and only use that particular alignment as the input to the distance measure. The idea comes in two flavors, domain dependent and domain independent.

In domain dependent landmarking, we attempt to find a single (or very few) fixed feature to use as a starting point for conversion of the shape to a time series. For example, in face profile recognition the most commonly used landmarks (fiducial points) are the chin or nose [5]. In limited domains this may be useful, but it requires building special purpose feature extractors. For example, even in a domain as intuitively well understood as human profiles, accurately locating the nose is a non-trivial problem, even if we discount the possibility of mustaches and glasses. Probably the only reason any progress has been made in this area is that most work reasonably assumes that faces presented in an image are likely to be upright. For shape matching in skulls, the canonical landmark is called the Frankfurt Horizontal [41], which is defined by the right and left porion (the highest point on the margin of the external auditory meatus) and the left orbitale (the lowest point on the orbital margin). However, a skull can be missing the relevant bones to determine this orientation and still have enough global information to match its shape to similar examples. Indeed the famous Skhul V skull shown in Figure 14 is such an example. Other examples of domain dependent landmarking include [39] who use the “*sharpest corner*” of leafs as landmarks. This idea appears meaningful in the subset of leaf shapes they considered, but in orbicular (circular) leafs the “*sharpest corner*” is not well defined.

In domain independent landmarking, we align all the shapes to some cardinal orientation, typically the major axis. This approach may be useful for the limited domains in which there is a well-defined major axis, perhaps the indexing of hand tools. However

¹ More precisely the time complexity is $O(Rp \log p)$, where p is the number of pixels in the perimeter and R is the number of rotations that need to be executed. Here $p = n$, and while R is a user defined parameter, it should be approximately equal n to guarantee all rotations (up to the limit of rasterization) are considered.

there is increasing recognition that the “...major axis is sensitive to noise and unreliable” [44]. For example a recent paper shows that under some circumstances, a single extra pixel can change the rotation by ± 90 degrees [45].

To show how brittle landmarking can be we performed a simple clustering experiment where we clustered three primate skulls using Euclidean distance with both the major axis technique, and the minimum distance of all possible rotations (as found by brute force). Figure 3 shows the result. It is clear that the major axes do not have any biological meaning: the points connecting each axis for each specimen are not homologous (of shared evolutionary origin). Therefore, the resulting cluster is meaningless in terms of biology and morphology [41].

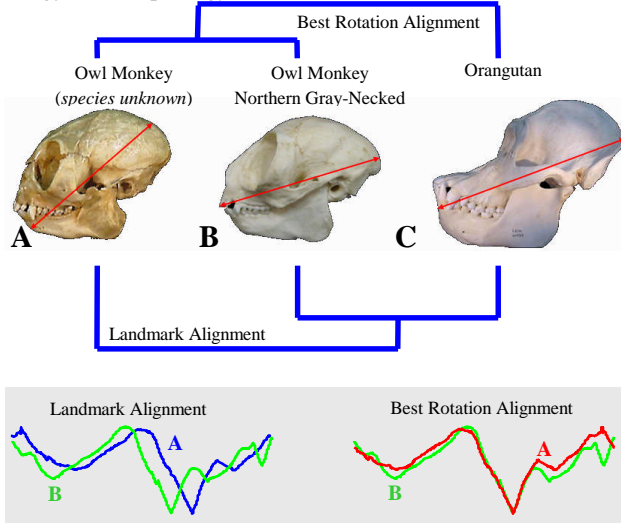


Figure 3: *Top*) Three primate skulls, two of them from the same genus, are clustered using both the landmark rotation beginning at the major axis, and the best rotation. *Bottom*) The landmark-based alignment of A and B explains why the landmark-based clustering is incorrect: a small amount of rotation error results in a large difference in the distance measure

Note that testing all rotations does not guarantee homology. However by considering all possible alignments, we would expect (under the principle of parsimony) to achieve an approximately homologous alignment. However, we note that what we are making claims here about subjective similarity, not morphogenesis [41].

The most important lesson we learned from this experiment (and dozens of other similar experiments on diverse domains [14]) is that rotation (mis)alignment is the most important invariance for shape matching, unless we have the best rotation then nothing else matters.

2.2 Rotation Invariant Features

A large number of papers achieve fast rotation invariant matching by extracting only rotation invariant features and indexing them with a feature vector [7]. This feature vector is often called the shapes “signature”. There are literally dozens of rotation invariant features including ratio of perimeter to area, fractal measures, elongatedness, circularity, min/max/mean curvature, entropy, perimeter of convex hull etc. In addition many researchers have attempted to frame the shape-matching problem as a more familiar histogram-matching problem. For example in [28] the authors build a histogram containing the distances between two randomly chosen points on the perimeter of the shapes in question. The

approach seems to be attractive, for example it can trivially also handle 3D shapes, however it suffers from extremely poor precision. For example, it cannot differentiate between the shapes of the lowercase letters “d” and “b”, or “p” and “q”, since these pairs of shapes have identical histograms. In general, all these methods suffer from very poor discrimination ability [7]. In retrospect this is hardly surprising. In order to achieve rotation invariance, all information that contains rotation information must be discarded; inevitably, some useful information may also be discarded in this process. Our experience with these methods suggests that they can be useful for making quick coarse discriminations, for example differentiating between skulls and vertebrae. However we could not get these methods to distinguish between the skulls of humans and orangutan, a trivial problem for human or the brute force algorithm discussed in the next section.

2.3 Brute Force Rotation Alignment

There are a handful of papers that recognize that the above attempts at approximating rotation invariance are unsatisfactory for most domains, and they achieve true rotation invariance by exhaustive brute force search over all possible rotations, but only at the expense of computational efficiency and indexability [1][2][3][9][23][39]. For example, paper [1] uses DTW to handle nonrigid shapes in the time series domain, while they note that most invariances are trivial to handle in this representation, they state “rotation invariance can (only) be obtained by checking all possible circular shifts for the optimal diagonal path.” This step makes the comparison of two shapes $O(n^3)$ and forces them to abandon hope of indexing. Similarly paper [39] notes “In order to find the best matching result, we have to shift one curve n times, where n is the number of possible start points.”

In [23] the authors discretize the shapes into chain codes, and introduce a fast dynamic programming method to test all rotations. They note “The algorithm runs in $O(nlgn)$ time, where n is the length of the compared strings.”. Of course this is an exact bound, but we achieve an empirical $O(n^{1.06})$ on large datasets (cf. Section 5). Given that most boundaries have about 1,000 datapoints long, this suggests that we are thousands of times faster while also able to avoid discretization errors and avoiding the need to set several parameters.

Dozens of papers have suggested that shape matching can be made faster by sampling the contours. For example, in [19] the authors note: “it is first necessary to reduce the number of data points on the contour to a reasonable number that can be evaluated using shape similarity measurement.” These authors are interested in classifying fish. The fish shapes are reduced down to mere forty data points because they “... found that a reduced data set of 40 points was sufficient to retain the important shape features for comparison” [19]. This dramatic data reduction did make the similarity measure more tractable, but we wondered if the assumption that it “retain(s) the important shape features” was true. We compared their results, which after considerable parameter tuning claimed “the highest recognition accuracy of 64%”, with rotation invariant Euclidean distance on the raw data. Surprisingly this simple, parameter-free method achieves 88.57% accuracy (cf Section 5), which is much greater than the sampling approach.

Other techniques introduced mitigate the untenable computational complexity of testing “all” rotations do so at the expense of introducing false dismissals. Typically they offer some implicit or explicit trick to find a one (or a small number of) of starting

point(s) [2][3][9]. For example paper [2] suggests “*In order to avoid evaluation of the dissimilarity measure for every possible pair of starting contour points ...we propose to extract a small set of the most likely starting points for each shape.*” Furthermore, both the heuristic used and the number of starting points must “*be adjusted to a given application*”, and it is not obvious how to best achieve this.

In forceful experiments on publicly available datasets it has been demonstrated that brute force rotation alignment produces the best precision/recall and accuracy in diverse domains [1][2]. In retrospect this is not too surprising. The rival techniques with rotation invariant features are all using some lossy transformation of the data. In contrast the brute force rotation alignment techniques are using a (potentially) lossless transformation of the data. With more high quality information to use, any distance measures will have an easier time reflecting the true similarity of the original images.

The contribution of this work is to speed up these accurate but slow methods by many orders of magnitude while producing identical results.

2.4 Indexing Star Light Curves

While this paper is focused on the indexing of shapes, it has come to our attention that our techniques are ideally suited to the indexing of an important type of astronomical data known as star light curves. We would be remiss not to make this connection clear, so we briefly discuss the application and provide some experimental results below.

Globally there are myriads of telescopes covering the entire sky and constantly recording massive amounts of valuable astronomical data. Having humans to supervise all observations is practically impossible; hence the increasing interest in computer aided astronomy. A star light curve is a time series of brightness of a celestial object as a function of time. The study of light curves in astronomy is associated with the study of variability of sources. That led to the discoveries of pulsars, extra solar planets, supernovae, the rate of expansion of the universe just to name few. At the Time Series Center at Harvard University Initiative in Innovative Computing there are more than a 100 million such curves (with billions more expected by 2009) however none of this data is currently searchable (other than by brute force search).

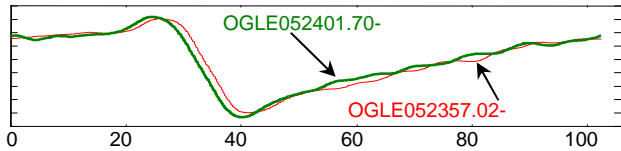


Figure 4: An examples of two similar star light curves.

There is a need to compare the similarity of light curves for basic astronomical research, for example in [29] researchers discover unusual light curves worthy of further examination by finding the examples with the least similarity to other objects. There are two things which make this difficult. First is the enormous volume of data, the second is the fact that while it is possible to extract a single period of a light curve, there is no natural starting point. In order to find the similarity of two light curves it is therefore necessary to compare every possible circular shift of the data [29], which as we show below corresponds exactly to the rotation invariance matching problem for shapes in the one-dimensional representation. The astronomical community [29] has mitigated some of the CPU effort for circular-shift matching by rediscovering the convolution “trick” long known to the shape

matching community [38]. However this technique does not help reduce disk accesses for data which does not fit in main memory, and only allows matching under the Euclidean metric.

3. ROTATION INVARIANT MATCHING

We begin by formally defining the rotation invariant matching problem. We begin by assuming the Euclidean distance, and generalize to other distance measures later. For clarity of presentation we will generally refer to “time series”, which the reader will note can be mapped back to the original shapes.

Suppose we have two time series, Q and C of length n , which were extracted from shapes by an arbitrary method.

$$Q = q_1, q_2, \dots, q_i, \dots, q_n$$

$$C = c_1, c_2, \dots, c_j, \dots, c_n$$

As we are interested in large data collections we denote a database of m such time series as \bar{Q} .

$$\bar{Q} = \{Q_1, Q_2, \dots, Q_m\}$$

If we wish to compare two time series, and therefore shapes, we can use the ubiquitous Euclidean distance:

$$ED(Q, C) \equiv \sqrt{\sum_{i=1}^n (q_i - c_i)^2}$$

When using Euclidean distance as a subroutine in a classification or indexing algorithm, we may be interested in knowing the exact distance only when it is eventually going to be less than some threshold r . For example, this threshold can be the “range” in range search or the “best-so-far” in nearest neighbor search. If this is the case, we can potentially speed up the calculation by doing early abandoning [17].

Definition 1. Early Abandon: During the computation of the Euclidean distance, if we note that the current sum of the squared differences between each pair of corresponding data points exceeds r^2 , then we can stop the calculation, secure in the knowledge that the exact Euclidean distance had we calculated it, would exceed r .

While the idea of early abandoning is fairly obvious and intuitive, it is so important to our work we illustrate it in Figure 5 and provide pseudocode in Table 1.

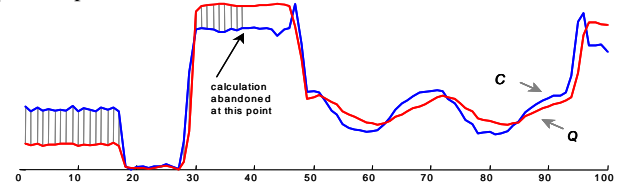


Figure 5: A visual intuition of early abandoning. Once the squared sum of the accumulated gray hatch lines exceeds r^2 , we can be sure the full Euclidean distance exceeds r

Note that the “num_steps” value returned by the optimized Euclidean distance in Table 1 is used only to tell us how useful the optimization was. If its value is significantly less than n this suggests dramatic speedup.

Table 1: Euclidean distance optimized with early abandonment

```

algorithm [dist, num_steps] = EA_Euclidean_Dist(Q, C, r)
accumulator = 0
for  $i = 1$  to length(Q)
    accumulator += (qi - ci)2
    if accumulator > r2

```

// Loop over time series
// Accumulate error contribution
// Can we abandon?


```

disp('doing an early abandon')
num_steps = i
return [infinity, num_steps] // Terminate and return an
end // infinite error to signal the
end // early abandonment.
return [sqrt(accumulator), length(Q)] // Terminate with true dist

```

While the Euclidean distance is a simple distance measure it produces surprisingly good results for clustering, classification and query by content of shapes, *if* the time series in question happen to be rotation aligned. For example, in an experiment in [30] we manually performed rotation alignment of the time series extracted from face profiles by explicitly showing the algorithm the beginning and endpoint of a face (the nape and Adams apple respectively).

However if the shapes are not rotation aligned, this method can produce extremely poor results. Recall the results in Figure 1, where a few degrees of misalignment give objectively and subjectively incorrect clusterings. To overcome this problem we need to hold one shape fixed, rotate the other, and record the minimum distance of all possible rotations.

For reasons that will become apparent later, we achieve this by expanding one time series into a matrix C of size n by n .

$$C = \begin{Bmatrix} c_1, c_2, \dots, c_{n-1}, c_n \\ c_2, \dots, c_{n-1}, c_n, c_1 \\ \vdots \\ c_n, c_1, c_2, \dots, c_{n-1} \end{Bmatrix}$$

Note that each row of the matrix is simply a time series, shifted (rotated) by one from its neighbors. It will be useful below to address the time series in each row individually, so we will denote the i^{th} row as C_i , which allows us to denote the matrix above in the more compact form of $C = \{C_1, C_2, \dots, C_n\}$.

We can now define the Rotation invariant Euclidean Distance (RED) as:

$$RED(Q, C) = \min_{1 \leq j \leq n} \left\{ ED(Q, C_j) \equiv \sqrt{\sum_{i=1}^n (q_i - c_i)^2} \right.$$

Table 2 shows the pseudocode to calculate this.

Table 2: An algorithm to find the rotated match between two time series

```

algorithm: [bestSoFar] = Test_All_Rotations(Q, C, r)
bestSoFar = r
for j = 1 to n
    distance = EA_Euclidean_Dist(Q, C_j, bestSoFar) // As in Table 1
    if distance < bestSoFar
        bestSoFar = distance;
    end;
end;
return [bestSoFar]

```

Note that the algorithm tries to take advantage of early abandoning by passing EA_Euclidean_Dist the value of r , the best rotation alignment discovered thus far.

If we are simply measuring the distance between two time series then the algorithm is invoked with r set to infinity, however, as we shall see below, if the algorithm is being used as a subroutine in a linear scan of a large dataset \bar{Q} , the calling routine can set the value of r to achieve speedup. In particular the calling function sets r to the value of the best match (under any rotation) discovered thus far. Table 3 shows the pseudocode. Note that the

time complexity for this algorithm is $O(mn^2)$. This is simply untenable for large datasets.

Table 3: An algorithm to find the best rotated match to query from a database of possible matches

```

algorithm: [best_match_loc, bestSoFar] = Search_Database_for_Rotated_Match(C, Q)
best_match_loc = null
bestSoFar = inf
for i = 1 to number_of_time_series_in_database(Q)
    distance = Test_All_Rotations(Q_i, C, bestSoFar); // As in Table 2
    if distance < bestSoFar
        best_match_loc = i
        bestSoFar = distance
    end;
end;
return [best_match_loc, bestSoFar]

```

We will review the notation introduced thus far in Table 4.

Table 4: Notation Table

C	A time series $c_1, c_2, \dots, c_j, \dots, c_n$
\mathcal{C}	A n by n matrix containing every rotation of C
C_i	The i^{th} row of the above
Q	Another time series $q_1, q_2, \dots, q_i, \dots, q_n$
\bar{Q}	A database containing many time series $\bar{Q} = \{Q_1, \dots, Q_m\}$

Note that our notation seems somewhat space inefficient in that it expands time series C , of length n , to a matrix of size n by n . However the rest of the database uses the original (arbitrary rotation) time series, and since the size of the database is assumed to be large, this overhead is asymptotically irrelevant.

There are two simple and useful generalizations of definitions thus far.

Mirror Image Invariance: Depending on the application we may wish to retrieve shapes that are enantiomorphic (mirror images) to the query. For example, in matching skulls, the best match may simply be facing the opposite direction. In contrast when matching letters we *don't* want to match a “d” to a “b”. If enantiomorphic invariance is required we can trivially achieve this by augmenting matrix C to contain C_i and $\text{reverse}(C_i)$ for $1 \leq i \leq n$.

Rotation-Limited Invariance: In some domains it may be useful to express *rotation-limited* queries. For example, in order to robustly retrieve examples of the number “6”, without retrieving examples of the number “9”, we can issue a query such as: “Find the best match to this shape allowing a maximum rotation of ± 15 degrees”. Our framework trivially supports such rotation-limited queries, by removing from the matrix C all time series that correspond to the unwanted rotations.

Thus far we have shown a brute force search algorithm that can support rotation invariance, rotation-limited invariance and/or mirror image invariance. We simply put the appropriate time series into matrix C and invoke the algorithm in Table 3. This algorithm, even though speeded up by the early abandoning optimization, is too slow for large datasets. In the next section we introduce our novel search mechanism.

4. WEDGE BASED ROTATION MATCHING

We will begin by showing how we can efficiently search for the best match in main memory. Since large datasets may not fit on disk we will further show how we can index the data.

4.1 Fast and Exact Main Memory Search

We begin by defining time series *wedges*. Imagine that we take several time series, C_1, \dots, C_k , from our matrix C . We can use these sequences to form two new sequences U and L :

$$U_i = \max(C_{1i}, \dots, C_{ki})$$

$$L_i = \min(C_{1i}, \dots, C_{ki})$$

U and L stand for Upper and Lower respectively. We can see why in Figure 6. They form the smallest possible bounding envelope that encloses all members of the set C_1, \dots, C_k from above and below. More formally:

$$\forall_i \quad U_i \geq C_{1i}, \dots, C_{ki} \geq L_i$$

For notational convenience, we will call the combination of U and L a *wedge*, and denote a wedge as W :

$$W = \{U, L\}$$

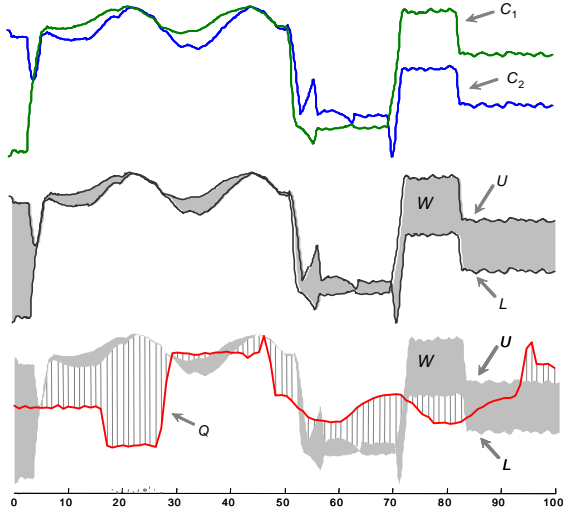


Figure 6: *Top*) Two time series C_1 and C_2 . *Middle*) A time series wedge W , created from C_1 and C_2 . *Bottom*) An illustration of LB_Keogh

We can now define a lower bounding measure between an arbitrary time series Q and the entire set of candidate sequences contained in a wedge W :

$$LB_Keogh(Q, W) = \sqrt{\sum_{i=1}^n \begin{cases} (q_i - U_i)^2 & \text{if } q_i > U_i \\ (q_i - L_i)^2 & \text{if } q_i < L_i \\ 0 & \text{otherwise} \end{cases}}$$

Below we show a proof of this lower bounding property. A similar proof appears in [14] and also in [21], where the authors use this representation for different problem.

Proposition 1: For any sequence Q of length n and a wedge W containing a set of time series C_1, \dots, C_k of the same length n , the following inequality holds:

$$LB_Keogh(Q, W) \leq ED(Q, C_s), \text{ where } s = 1, 2, \dots, k.$$

Proof:

Suppose we know that among the k time series C_1, \dots, C_k , C_s has the minimal Euclidean distance to query Q . And we wish to prove

$$\sqrt{\sum_{i=1}^n \begin{cases} (q_i - U_i)^2 & \text{if } q_i > U_i \\ (q_i - L_i)^2 & \text{if } q_i < L_i \\ 0 & \text{otherwise} \end{cases}} \leq \sqrt{\sum_{i=1}^n (q_i - C_{si})^2}$$

Since the terms under radicals are positive, we can square both sides:

$$\sum_{i=1}^n \begin{cases} (q_i - U_i)^2 & \text{if } q_i > U_i \\ (q_i - L_i)^2 & \text{if } q_i < L_i \\ 0 & \text{otherwise} \end{cases} \leq \sum_{i=1}^n (q_i - C_{si})^2$$

Below we will show that every term in the left summation can be matched with some greater or equal term in the right summation.

There are three cases to consider, for the moment we will just consider the case when $q_i > U_i$. We want to show:

$$(q_i - U_i)^2 \leq (q_i - C_{si})^2$$

$$(q_i - U_i) \leq (q_i - C_{si})$$

$$-U_i \leq -C_{si}$$

$$C_{si} \leq U_i$$

$$C_{si} \leq \max(C_{1i}, \dots, C_{ki})$$

This is obviously true.

The case $q_i < L_i$ yields to a similar argument. The final case is simple to show, since clearly $0 \leq (q_i - C_{si})^2$ because $(q_i - C_{si})^2$ must be nonnegative.

Thus we have shown that each term on the left side is matched with an equal or larger term on the right side. Our inequality holds. ■

Note that the LB_Keogh function has been used before to support DTW [16][30][31][37], uniform scaling [18], and query filtering [40]. For these tasks the lower bounding distance function is the same, but the definition of U and L are different.

There are two important observations about LB_Keogh. First, in the special case where W is created from a single candidate sequence, it degenerates to the Euclidean distance. Second, not only does LB_Keogh lower bound all the candidate sequences C_1, \dots, C_k , but we can also do *early abandon* with LB_Keogh. While the latter fact might be obvious, for clarity we make it explicit in Table 5.

Table 5: LB_Keogh optimized with early abandonment

```

algorithm [dist, num_steps] = EA_LB_Keogh(Q, W, r)
accumulator = 0
for i = 1 to length(Q) // Loop over time series
  if q_i > W.U_i // Accumulate error contribution
    accumulator += (q_i - W.U_i)^2
  elseif q_i < W.L_i
    accumulator += (q_i - W.L_i)^2
  end
  if accumulator > r^2 // Can we abandon?
    return [infinity, i] // Terminate and return an infinite error
  end // to signal the early abandonment.
end
return [sqrt(accumulator), length(Q)] // Terminate with true dist

```

Note once again that the value returned in “num_steps” is merely a bookkeeping device to allow a post mortem evaluation of efficiency.

Suppose we have just two time series C_1 and C_2 of length n , and we know that in future we will be given a time series query Q and asked if one (or both) of C_1 and C_2 are within r of the query. We naturally wish to minimize the number of steps we must perform (“steps” are measured by “num_steps”). We are now in a position to outline two possible approaches to this problem.

- We can simply compare the two sequences, C_1 and C_2 (in either order) to the query using the early abandon algorithm introduced in Table 1. We will call this algorithm, *classic*.
- We can combine the two candidate sequences into a wedge, and compare Q to the wedge using LB_Keogh . If the LB_Keogh function early abandons, we are done. We can say with absolute certainty that neither of the two candidate sequences is within r of the query. If we cannot early abandon on the wedge, we need to individually compare the two candidate sequences, C_1 and C_2 (in either order) to the query. We will call this algorithm, *Merge*.

Let us consider the best and worst cases for each approach. For *classic* the worst case is if both candidate sequences are within r of the query, which will require $2n$ steps. In the best case, the first point in the query may be radically different to the first point in either of the candidates, allowing immediate early abandonment and giving a total cost of 2 steps.

For *Merge*, the worst case is also if both candidate sequences are within r of the query, because we will waste n steps in the lower bounding test between the query and the wedge, and then n steps for each individual candidate, for a total of $3n$. However the best case, also if the first point in the query is radically different, would allow us to abandon with a total cost of 1 step.

Which of the two approaches is better depends on:

- The shapes of C_1 and C_2 . If they are similar, this greatly favors *Merge*.
- The shape of Q . If Q is truly similar to one (or both) of the candidate sequences, this would greatly favor *classic*.
- The matching distance r . Here the effect is non monotonic and dependent on the two factors above.

We can generalize the notion of wedges by hierarchically nesting them. Let us begin by augmenting the notation of a wedge to include information about the sequences used to form it. For example, if a wedge is built from C_1 and C_2 , we will denote it as $W_{(1,2)}$. Note that a single sequence is a special case of a wedge, for example the sequence C_1 can also be denoted as W_1 . We can combine $W_{(1,2)}$ and W_3 into a single wedge by finding maximum and minimum values for each i^{th} location, from *either* wedge. More concretely:

$$\begin{aligned}
 U_i &= \max(W_{(1,2)i}, W_{3i}) \\
 L_i &= \min(W_{(1,2)i}, W_{3i}) \\
 W_{((1,2),3)} &= \{U, L\}
 \end{aligned}$$

In Figure 7 we illustrate this notation. We call $W_{(1,2)}$ and W_3 *children* of wedge $W_{((1,2),3)}$. Since individual sequences are special cases of wedges, we can also call C_1 and C_2 children of $W_{(1,2)}$.

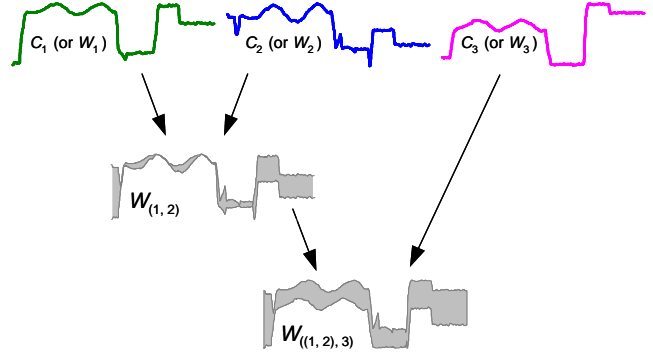


Figure 7: An illustration of hierarchically nested wedges

Given the generalization to hierarchal wedges, we can now also generalize the *Merge* approach. Suppose we have a time series Q and a wedge $W_{((1,2),3)}$. We can compare the query to the wedge using LB_Keogh . If the LB_Keogh function early abandons, we are done. We know with certainty that none of the three candidate sequences is within r of Q . If we cannot early abandon on the wedge, we need to compare the two child wedges, $W_{(1,2)}$ and W_3 to the query. Again, if we cannot early abandon on the wedge $W_{(1,2)}$, we need to individually compare the two candidate sequences, C_1 and C_2 (in either order) to the query. We call this algorithm *H-Merge* (Hierarchal Merge).

The utility of a wedge is strongly correlated to its area. We can get some intuition as to why by visually comparing $LB_Keogh(Q, W_{(1,2)})$ with $LB_Keogh(Q, W_{((1,2),3)})$ as shown in Figure 8. Note that the area of $W_{((1,2),3)}$ is much greater than that of $W_{(1,2)}$, and that this reduces the value returned by the lower bound function and thus the possibility to early abandon.

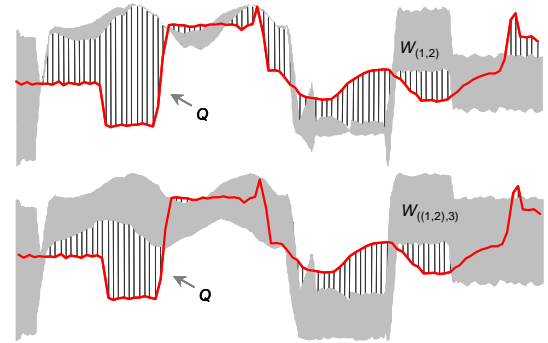


Figure 8: *Top*) An illustration of $LB_Keogh(Q, W_{(1,2)})$. *Bottom*) An illustration of $LB_Keogh(Q, W_{((1,2),3)})$. Note that the tightness of the lower bound is proportion to the number and length of vertical lines

For some problems, the *H-Merge* algorithm can give exceptionally poor performance. If the wedge $W_{(1,2)}$, created from C_1 and C_2 has an exceptional large area (i.e. C_1 and C_2 are very dissimilar), it is very unlikely to be able to prune off any steps.

At this point we can see that the efficiency of *H-Merge* is dependent on the candidate sequences and Q itself. In general, merging similar sequences into a hierarchal wedge is a good idea, but merging dissimilar sequences is a bad idea.

The observations above motivate a final generalization of *H-Merge*. Recall that to achieve rotation invariance we expanded our time series C into a matrix with n time series. Given these n sequences, we can merge them into K hierarchal wedges, where $1 \leq K \leq n$. This merging forms a partitioning of the data, with each sequence

belonging to exactly one wedge. We will use \mathbf{W} to denote a set of hierarchal wedges:

$$\mathbf{W} = \{W_{\text{set}(1)}, W_{\text{set}(2)}, \dots, W_{\text{set}(K)}\}, \quad 1 \leq K \leq n$$

where $W_{\text{set}(i)}$ is a (hierarchically nested) subset of the n candidate sequences. Note that we have

$$W_{\text{set}(i)} \cap W_{\text{set}(j)} = \emptyset \text{ if } i \neq j, \text{ and}$$

$$|W_{\text{set}(1)} \cup W_{\text{set}(2)} \cup \dots \cup W_{\text{set}(K)}| = n$$

We will attempt to merge together only similar sequences. We can then compare this set of wedges against our query. Table 6 formalizes the algorithm.

Table 6: Algorithm *H-Merge*

```

algorithm [dist] = H-Merge( $Q, \mathbf{W}, K, r$ )
 $S = \{\text{empty}\}$  // Initialize a stack.
for  $i = 1$  to  $K$  // Place all the wedges into the stack.
    enqueue( $W_{\text{set}(i)}, S$ )
end
while not empty( $S$ )
     $T = \text{dequeue}(S)$ 
     $\text{dist} = \text{EA\_LB\_Keogh}(Q, T, r)$  // Note that is early abandon version.
    if isfinite( $\text{dist}$ ) // We did not early abandon.
        if cardinality( $T$ ) = 1 //  $T$  was an individual sequence.
            disp('The sequence ',  $T$ , ' is ',  $\text{dist}$ , ' units from the query')
            return[ $\text{dist}$ ]
        else //  $T$  was a wedge, find its children
            enqueue(children( $T$ ),  $S$ ) // and push them onto the stack.
        end
    end
end

```

Note that this algorithm is designed to replace the **Test_All_Rotations** algorithm that is invoked as a subroutine in the **Search_Database_for_Rotated_Match** algorithm shown in Table 3.

As we shall see in our empirical evaluations, *H-Merge* can produce very impressive speedup if we make judicious choices in the set of hierarchal wedges that make up \mathbf{W} . However, the number of possible ways to arrange the hierarchal wedges is greater than K^K , and the vast majority of these arrangements will be very poor, so specifying a good arrangement of \mathbf{W} is critical.

A simple observation alleviates the need to invent a new algorithm to find a good arrangement of \mathbf{W} . Note that hierarchal clustering algorithms have very similar goals to an ideal wedge-producing algorithm. In particular, hierarchal clustering algorithms can be seen as attempting to minimize the distances between objects in each subtree. A wedge-producing algorithm should attempt to minimize the area of each wedge. However the area of a wedge is simply the maximum Euclidean distance between any sequences contained therein (i.e Newton-Cotes rule from elementary calculus). This motivates us to derive wedge sets based on the result of a hierarchal clustering algorithm. Figure 10 shows wedge sets \mathbf{W} , of every size from 1 to 5, derived from the dendrogram shown in Figure 9.

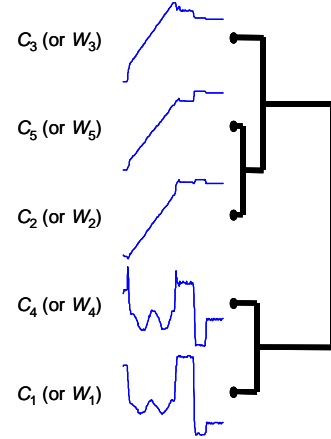


Figure 9: A dendrogram of five sequences C_1, C_2, \dots, C_5 , clustered using group average linkage

Given that the clustering algorithm produces the tentative wedge sets, all we need to do is to choose the best one. We could attempt to do this by eye, for example in Figure 10 it is clear that any sequence that early abandons on W_3 , will almost certainly also early abandon on both W_2 and W_5 ; similar remarks apply to W_1 and W_4 . At the other extreme, the wedge at $K = 1$ is so “fat” that it is likely have poor pruning power. The set $\mathbf{W} = \{W_{((2,5),3)}, W_{(1,4)}\}$ is probably the best compromise. However because the set of time series might be very large, such visual inspection is not scalable.

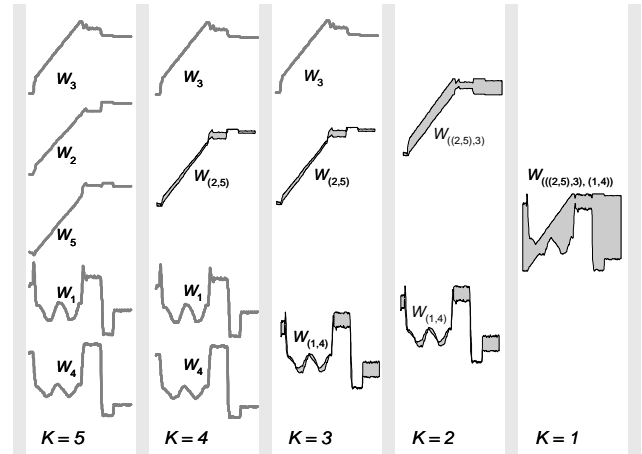


Figure 10: Wedge sets \mathbf{W} , of size 1 to 5, derived from the dendrogram shown in Figure 9

The problem is actually even more complex, in that the best value for K also depends on the current value of r (Recall r is the “best-so-far” in nearest neighbor search.). If r is large then very little early abandoning is possible and this favors a large value for K . In contrast, if r is small we can do a lot of early abandoning, and we are better off having many sequences in a single wedge so we can early abandon all of them with a single calculation. Note however that for nearest neighbor search the value of r will get smaller as we search through the database.

With this in mind, we dynamically choose the wedge set based on a fast empirical test. We start with the wedge set where $K = 2$. Each time the **bestSoFar** value changes, we test a subset of the possible values of K and choose the most efficient one (as measured by **num_steps**) as the next K to use. Which subset to test

is decided on-the-fly based on the current K value. They are the values which evenly divide the ranges [1, current_K] and [current_K, max_K] into 5 intervals. Note that on average the **bestSoFar** value only changes $\log(m)$ during a linear search, so this slight overhead in adjusting the parameter is not too burdensome, however we do include this cost in all experiments in Section 5.

4.2 Lower Bounding in Index Space

True rotation invariance has traditionally been so demanding in terms of CPU time that little or no effort was made to index it (or it was indexed with the possibility of false dismissals with regard to the raw shapes [4]). As we shall see in the experiments in Section 5.2, the ideas presented in the last section produce such dramatic reductions in CPU time that it is worth considering indexing the data.

There are several possible techniques we could consider for indexing. Recent years have seen dozens of papers on indexing time series envelopes that we could attempt to leverage off [16][21][30][31][37]. The only non-trivial adaptation to be made is that instead of the query being a single envelope, it would be necessary to search for the best match to K envelopes in the wedge set \mathbf{W} .

Note however that we do not necessarily have to use the enveloping idea in the indexing phase. So long as we can lower bound in the index space we can use an arbitrary technique to get (hopefully a small subset of) the data from disk to main memory [8], where our *H-Merge* can very efficiently find the distance to the best rotation.

Table 7: A Vantage Point Tree for Indexing Shapes

```

Algorithm [BSF] = NNSearch(C)
BSF.ID = null; // BSF is the Best-So-Far variable
BSF.distance = infinity;
W = convert_time_series_to_wedge_set(C);
Search(Qroot, W, BSF); // Invoke subroutine on the root of index tree
Subroutine Search(NODE, W, BSF)
if NODE.isLeaf // we are at a leaf node.
for each compressed time-series cT in node
LB = computeLowerBound(cT, W);
queue.push(cT, LB); // sorted by lower bound.
end
while (not (queue.empty()) and (queue.top().LB < BSF.distance))
if (BSF.distance > queue.top().LB)
retrieve full time series Q of queue.top() from disk;
distance = H-Merge(Q, W, BSF.distance) // calculate full distance.
if distance < BSF.distance // update the best-so-far
BSF.distance = distance; // distance and location.
BSF.ID = Q;
end
end
end
else // we are at a vantage point.
LB = computeLowerBound(VP, W);
queue.push(VP, LB);
if LB < (node.median + BSF.distance)
search(NODE.left, W, BSF); // recursive search left.
else
search(NODE.right, W, BSF); // recursive search right.
end
end
end

```

One possible method to achieve this indexable lower bound is to use Fourier methods. Many authors have independently noted that transforming the signal to the Fourier space and calculating the Euclidean distance between the *magnitude* of the coefficients produces a lower bound to any rotation [4][38]. We can leverage of this lower bound to use a VP-tree to index our time series as shown in Table 7.

This technique is adapted from [38], and we refer the reader to this work for a more complete treatment.

4.3 Generalizing to other Distance Measures

As we shall see in Section 5, the Euclidean distance is typically very effective and intuitive as a distance measure for shapes. However in some domains it may not produce the best possible precision/recall or classification accuracy [2][30]. The problem is that even after best rotation alignment, subjectively similar shapes may produce time series that are globally similar but contain local “distortions”. These distortions may correspond to local features in that are present in both shapes but in different proportions. For example in Figure 11 we can see that the larger brain case of the Lowland Gorilla changes the locations in which the brow ridge and jaw map to in a time series relative to the Mountain Gorilla.

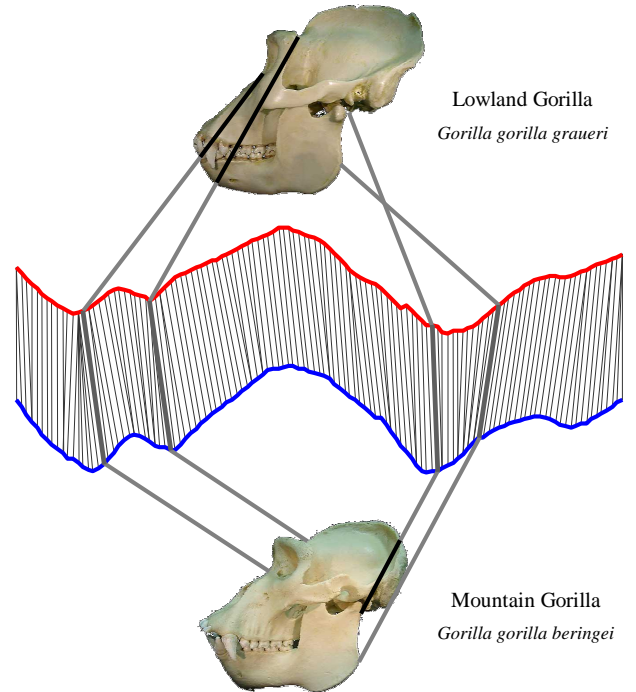


Figure 11: The Lowland Gorilla and Mountain Gorilla are morphologically similar, but have slightly different proportions. Dynamic Time Warping can be used to align homologous features in the time series representation space

Even if we assume that the database contains the actual object used as a query, it is possible that the two time series are distorted versions of each. Here the distortions may be caused by camera perspective effect, differences in lighting causing shadows which appear to be features, parallax etc.

Fortunately there is a well-known technique for compensating such local misalignments, Dynamic Time Warping (DTW) [16][30]. While DTW was invented in the context of 1D speech signals others have noted its utility for matching shapes, including face profiles [5], hand gestures [25], leaves [30] and handwriting [31].

To align two sequences using DTW, an n -by- n matrix is constructed, where the $(i^{\text{th}}, j^{\text{th}})$ element of the matrix is the distance $d(q_i, c_j)$ between the two points q_i and c_j (i.e. $d(q_i, c_j) = (q_i - c_j)^2$). Each matrix element (i, j) corresponds to the alignment between the points q_i and c_j , as illustrated in Figure 12.

A warping path P is a contiguous set of matrix elements that defines a mapping between Q and C . The i^{th} element of P is defined as $p_i = (i, j)$, so we have:

$$P = p_1, p_2, \dots, p_t, \dots, p_T \quad n \leq T < 2n-1$$

The warping path that defines the alignment between the two time series is subject to several constraints. For example, the warping path must start and finish in diagonally opposite corner cells of the matrix; the steps in the warping path are restricted to adjacent cells (including diagonally adjacent cells); the points in the warping path must be monotonically spaced in time. In addition to these constraints, virtually all practitioners using DTW also constrain the warping path in a global sense by limiting how far it may stray from the diagonal [16][30][31]. A typical constraint is the Sakoe-Chiba Band which states that the warping path cannot deviate more than R cells from diagonal [34].

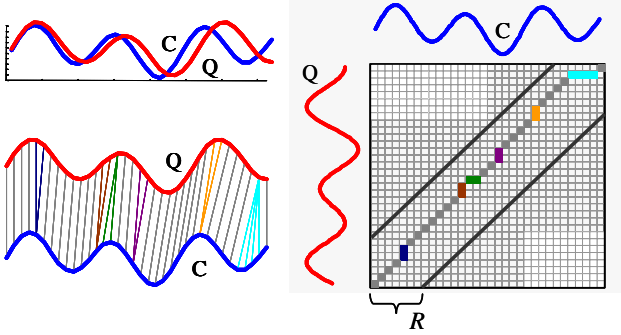


Figure 12: *Left*) Two time series sequences with local differences. *Right*) To align the sequences we construct a warping matrix, and search for the optimal warping path, shown with solid squares. Note that Sakoe-Chiba Band with width R is used to constrain the warping path

The optimal warping path can be found in $O(nR)$ time by dynamic programming [16].

Based on an arbitrary wedge W and the allowed warping range R , we define two new sequences, DTW_U and DTW_L :

$$DTW_U_i = \max(U_{i-R} : U_{i+R})$$

$$DTW_L_i = \min(L_{i-R} : L_{i+R})$$

They form an additional envelope above and below the wedge, as illustrated in Figure 13.

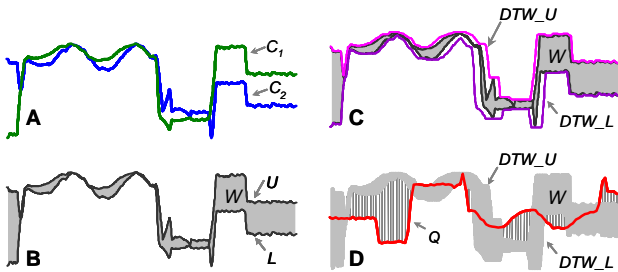


Figure 13: The idea of bounding envelopes introduced in Figure 6 is generalized to allow DTW. **A**) Two time series C_1 and C_2 . **B**) A time series wedge W , created from C_1 and C_2 . **C**) In order to allow lower bounding of DTW, an additional envelope is created above and below the wedge. **D**) An illustration of LB_Keogh_{DTW}

We can now define a lower bounding measure for DTW distance between an arbitrary query Q and the entire set of candidate sequences contained in a wedge W :

$$LB_Keogh_{DTW}(Q, W) = \sqrt{\sum_{i=1}^n \begin{cases} (q_i - DTW_U_i)^2 & \text{if } q_i > DTW_U_i \\ (q_i - DTW_L_i)^2 & \text{if } q_i < DTW_L_i \\ 0 & \text{otherwise} \end{cases}}$$

We will now prove the claim of the lower bounding.

Proposition 2: For any sequence Q of length n and a wedge W containing a set of time series C_1, \dots, C_k of the same length n , for any global constraint on the warping path of the form $j-R \leq i \leq j+R$, the following inequality holds:

$$LB_Keogh_{DTW}(Q, W) \leq DTW(Q, C_s), \text{ where } s = 1, 2, \dots, k.$$

Proof:

Suppose we know that among the k time series C_1, \dots, C_k , C_s has the minimal DTW distance to query Q . And we wish to prove

$$\sqrt{\sum_{i=1}^n \begin{cases} (q_i - DTW_U_i)^2 & \text{if } q_i > DTW_U_i \\ (q_i - DTW_L_i)^2 & \text{if } q_i < DTW_L_i \\ 0 & \text{otherwise} \end{cases}} \leq \sqrt{\sum_{i=1}^n p_{st}}$$

Since the terms under radicals are positive, we can square both sides:

$$\sum_{i=1}^n \begin{cases} (q_i - DTW_U_i)^2 & \text{if } q_i > DTW_U_i \\ (q_i - DTW_L_i)^2 & \text{if } q_i < DTW_L_i \\ 0 & \text{otherwise} \end{cases} \leq \sum_{i=1}^n p_{st}$$

Recall that that when we stated the definition of the warping path above we had, $P = p_1, p_2, \dots, p_t, \dots, p_T \quad n \leq T < 2n-1$. We therefore have $n \leq T$, so our strategy will be to show that every term in the left summation can be matched with some greater or equal term in the right summation.

There are three cases to consider, for the moment we will just consider the case when $q_i > DTW_U_i$. We want to show:

$$(q_i - DTW_U_i)^2 \leq p_{st}$$

$$(q_i - DTW_U_i)^2 \leq (q_i - C_{sj})^2 \quad \text{By Definition 3}$$

$$(q_i - DTW_U_i) \leq (q_i - C_{sj})$$

Since $q_i > DTW_U_i$, we can take square roots on both sides

$$-DTW_U_i \leq -C_{sj}$$

Subtract q_i from both sides

$$C_{sj} \leq DTW_U_i$$

Add $DTW_U_i + C_{sj}$ to both sides

$$C_{sj} \leq \max(U_{i-R} : U_{i+R})$$

By definition $DTW_U_i = \max(U_{i-R} : U_{i+R})$

Since the query sequence Q and all the candidate sequences C_1, \dots, C_k are of the same length and $j-R \leq i \leq j+R$, we know $i-R \leq j \leq i+R$. So we can rewrite the right side and the inequality becomes

$$C_{sj} \leq \max(U_{i-R}, U_{(i+1)-R}, \dots, U_j, \dots, U_{i+R})$$

If we remove all terms except U_j from the RHS we are left with $C_{sj} \leq \max(U_j)$ which is obviously true since $U_j = \max(C_{1j}, \dots, C_{kj})$.

The case $q_i < DTW_U_i$ yields to a similar argument. The final case is simple to show, since clearly $0 \leq (q_i - C_{sj})^2$ because $(q_i - C_{sj})^2$ must be nonnegative.

Thus we have shown that each term on the left side is matched with an equal or larger term on the right side. Our inequality holds. ■

For brevity we omit the very minor modifications required to index $LB_Keogh_{DTW}(Q,W)$, however [37] contains the necessary modifications for both DTW and for LCSS which is discussed below.

To facilitate later efficiency comparisons to Euclidean distance and other methods, it will be useful to define the time complexity of DTW in terms of “num_steps” as returned by Table 1 and Table 5. The variable “num_steps” is the number of real-value subtractions that must be performed, and completely dominates the CPU time, since the square root function is only performed once (and can be removed, see [17]). If we construct a full n by n warping matrix, then DTW clearly requires at least n^2 steps. However as we noted above and illustrated in Figure 12, we can truncate the corners of the matrix to reduce this number to approximately nR , where R is the width of the Sakoe-Chiba Band. While nR is the number of steps for a single DTW, we expect the average number of steps to be less, because some full DTW calculations will not be needed if the lower bound test fails. Since the lower bound test requires n steps, the average number of steps when doing m comparisons should be:

$$\frac{m*a(nR) + m(n)}{m}$$

Where a is the fraction of the database that requires the full DTW calculated. Note that even this is pessimistic, since both DTW^2 and LB_Keogh_{DTW} are implemented as early abandoning (recall Table 5). We therefore simply count the “num_steps” required by each approach and divide it by m to get the average number of steps required for one comparison.

In addition to DTW, several researchers have suggested using Longest Common SubSequence (LCSS) as a distance measure for shapes. The LCSS is very similar to DTW except that while DTW insists that every point in C maps onto one (or more) point(s) in Q , LCSS allows some points to go unmatched. The intuition behind this idea in a time series domain is that subsequences may contain additions or deletions, for example an extra (or forgotten) dance move in a motion capture performance, or a missed beat in ECG data. Rather than forcing DTW to produce an unnatural alignment between two such sequences, we can use LCSS, which simply ignores parts of the time series that are too difficult to match. In the image space the missing section of the time series may correspond to a partial occlusion of an object, or to a physically missing part of the object, as shown in Figure 14.

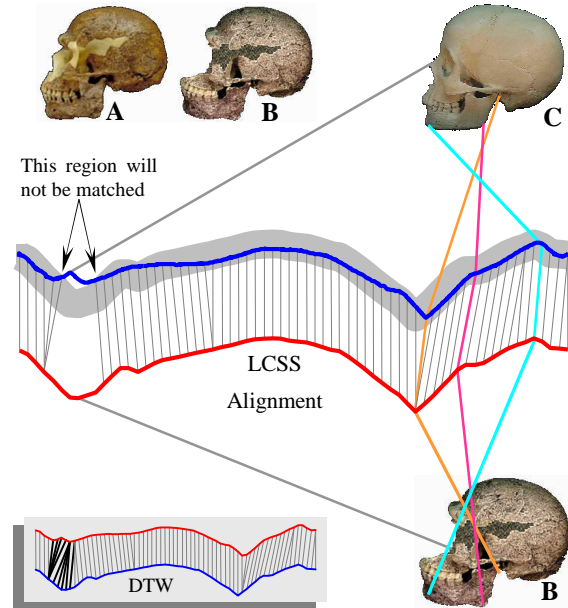


Figure 14: **A)** The famous Skul V is generally reproduced with the missing bones extrapolated in epoxy, however the original Skul V (**B**) is missing the nose region, which means it will match to a modern human (**C**) poorly, even after DTW alignment (inset). In contrast, LCSS alignment will not attempt to match features that are outside a “matching envelope” (heavy gray line) created from the other sequence.

Real world examples of domains that require LCSS abound. For example anthropologists are interested in exploring large dataset of projectile points (“arrowheads”). At the UCR Lithic Technology Lab at UCR there are over a million specimens, so indexing is required for efficient access. While anthropologists have long been interested in shape, interest in matching such objects is further fueled by the availability of computing power and by a recent movement that notes, “an increasing number of archaeologists are showing interest in employing Darwinian evolutionary theory to explain variation in the material record” [26]. Anthropologists have recently used tools from biological morphology to attempt to explain spatial and temporal distribution of projectile points in North America. As we illustrate in Figure 15 many examples are incomplete, missing tip or tangs. LCSS can ignore such missing feature to provide more robust matching.

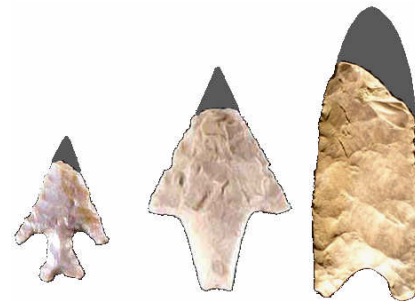


Figure 15: Project points are frequently found with broken tips or tangs. Such objects require LCSS to find meaningful matches to complete specimens. From left to right, Edwards, Langtry, and Golondrina projectile points.

² Note that a *recursive* implementation of DTW would always require nR steps, however *iterative* implementation (as used here) can potentially early abandon with as few as R steps.

While we considered LCSS for generality, we will not further explain how to incorporate it into our framework. It has been

shown in [37] that it is trivial to lower bound LCSS using the envelope-based techniques described above. The minor changes include reversing some inequality signs since LCSS is a similarity measure, not a distance measure. Unlike Euclidean distance which has no parameters, or DTW, which has one intuitive and easy to set parameter, LCSS requires 2 parameters, and tuning them is nontrivial. In objective classification experiments we found that we could sometimes tune LCSS to *slightly* beat DTW on *some* problems, however we did not have large enough datasets to allow training/test splits that guarded against overfitting to a statistically significant standard. Automatically choosing the correct parameters for LCSS is a matter for future research.

5. EXPERIMENTAL RESULTS

In this section we empirically evaluate our approach. We begin by stating our experimental philosophy. In a recent paper Veltkamp and Latecki attempted to reproduce the accuracy claims of several shape matching papers but discovered to their dismay that they could not match the claimed accuracy for any approach [36]. One suggested reason is the observation that many approaches have highly tuned parameters, a fact which we believe makes Euclidean distance (zero parameters) and DTW (one parameter) particularly attractive. Veltkamp and Latecki conclude “*It would be good for the scientific community if the reported test results are made reproducible and verifiable by publishing data sets and software along with the articles*”. We completely concur and have placed all datasets at the following URL [14].

5.1 Effectiveness of Shape Matching

In general this paper is not making any claims about the *effectiveness* of shape matching. Because we are simply speeding up arbitrary distance calculations on arbitrary 1-dimensional representations of shapes, we automatically inherit the well-documented effectiveness of other researchers published work [1][2][3][9][12][30][38].

Nevertheless, for completeness and in order to justify the extra computational expense of DTW, we will show the effectiveness of shape matching on several publicly available datasets.

Table 8 shows the error rate of one-nearest neighbor classification as measured using leaving-one-out evaluation. Recall that Euclidean distance has no parameters, DTW has a single parameter (the warping window width R) which was learned by looking only at the training data.

Table 8: The Error of Euclidean distance and DTW on publicly available datasets

Name	Number of Classes	Number of Instances	Euclidean Error (%)	DTW Error (%) { R }
Face	16	2240	3.839%	3.170% {3}
Swedish Leaves	15	1125	13.33%	10.84% {2}
Chicken	5	446	19.96%	19.96% {1}
MixedBag	9	160	4.375%	4.375% {1}
OSU Leaves	6	442	33.71%	15.61% {2}
Diatoms	37	781	27.53%	27.53% {1}
Aircraft	7	210	0.95%	0.0% {3}
Fish	7	350	11.43%	9.71% {1}
Light-Curve	3	954	14.15%	11.43% {3}
Yoga	2	3300	4.70%	4.85% {1}

For the Face and Leaf datasets the (approximate) correct rotation was known [30]. We removed this information by randomly rotating the images.

The MixedBag dataset is small enough to run the more computationally expensive Chamfer [6] and Hausdorff [27] distance measures. They achieved an error rate of 6.0% and 7.0% respectively [38], slightly worse than Euclidean distance. Likewise the Chicken dataset allows us to compare directly to [24], which used identical experiments to test 6 different algorithms based on *discrete* sequences extracted from the shapes. The best of these algorithms had an error rate of 20.5% and took over a minute for each distance calculation, whereas our approach takes an average time of 0.0039 seconds for each distance calculation³. For the Diatom dataset, the results are competitive with human experts, whose error rates ranged from 57% to 13.5% [12], and only slightly worse than the Morphological Curvature Scale Spaces (MCSS) approach of [12], which got 26.0%. Note however that the Euclidean distance requires zero parameters once the time series have been extracted, whereas the MCSS has several parameters to set. On the aircraft dataset the data donors tried 4 different Hidden Markov Model based approaches and achieve a *best* error-rate of 0.95% [35]. However, we can achieve this accuracy with zero-parameter Euclidean distance and get zero error with DTW. The data donors of the fish dataset tested many shape descriptors, such as Fourier descriptors, polygon approximation and line segments to achieve the best error rate of 36.0% [19], however we get dramatically lower error rates for both Euclidean distance and DTW.

The yoga dataset is of particular interest. It has previously been classified *without* rotation invariance [15]. In that case human volunteers painstakingly located a landmark point in each of 3,300 images. The accuracy for the human annotated dataset was 17.0% and 15.5% for Euclidean distance and DTW respectively. However the rotation invariant classification here has reduced the error rate by a factor of three. Since the only thing to differ between the two experiments is rotation invariance, this strongly supports the contention made in Section 2.1, that “*rotation (mis)alignment is the most important invariance for shape matching, unless we have the best rotation then nothing else matters*”. Note that here DTW is very slightly worse on the dataset, but the difference is not statistically significant at the 0.01 level.

5.2 Shape Matching Sanity Checks

In general the experiments in the previous section show two things (which had been noted before), the extra effort of DTW is useful in some domains, and very simple time series representations of shapes are complete to other more complex representations.

We also performed extensive “sanity check” experiments in domains where we could meaningful visualize the results.

Our first example uses a large database of skulls. For all primate species where we have at least two examples we perform a hierarchical clustering and check to see if both samples of the same species clustered together. Figure 16 shows a typical example.

³ We are aware that one should normally not compare CPU times from different computers, however here the 4 orders of magnitude offers a comfortable margin that dwarfs implementation details.

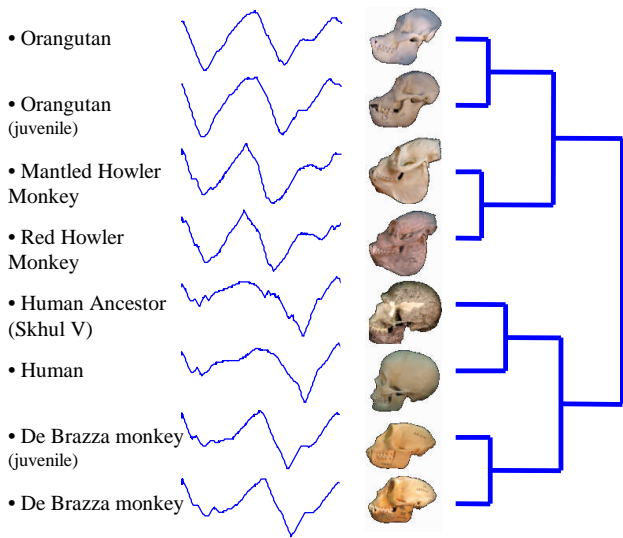


Figure 16: A group average hierarchical clustering of eight primate skulls based on the lateral view, using Euclidean distance

It is important to recall that Figure 16 shows a phenogram, *not* a phylogenetic tree. However on larger scale experiments in this domain (shown in [14]) we found that large subtrees of the dendrograms did conform to the current consensus on primate evolution.

While the Euclidean distance works very well on the relatively simple primate skulls, we found that considering a more (morphologically) diverse groups of animals, such as all reptiles, requires DTW as a distance measure. Consider Figure 17 which shows a hierarchical clustering of a very diverse set of reptiles. As with the primates, this is not the correct phylogenetic tree for these animals, once again however, the (uniquely colored) subtrees do correspond to current consensus on reptiles evolution based on DNA analysis and/or more complete morphological studies [10][11].

Note that we are *not* claiming that our shape matching techniques replace or even complement classic morphometrics in zoology. The point of these experiments is that if the shape matching techniques can produce intuitive results in a domain in which we know the correct relationships by other means, this suggests that algorithms may also produce meaningful results in shape problems for which there is more uncertainty, including projectile points (see [26] and Figure 15), petroglyphs, insect bite patterns in leaves [42], mammographic calcifications [43] etc.

It has recently been claimed that shape matching methods that only look at the contours of shapes (boundary based methods) are brittle to articulation distortion [33], however we believe that while this may be true for certain boundary based methods (i.e Hausdorff, Champer etc) the centroid based method we use is *very* robust to articulation distortions. To demonstrate this, we conducted a simple experiment/demonstration. We took three Lepidoptera, including the very similar and closely related *Actias maenaes* and *Actias philippinica*, and produced a copy of each. We then took these copies and “bent” the right hindwing. The clustering of the three originals and three copies under Euclidean distance, group average linkage is shown in Figure 18.

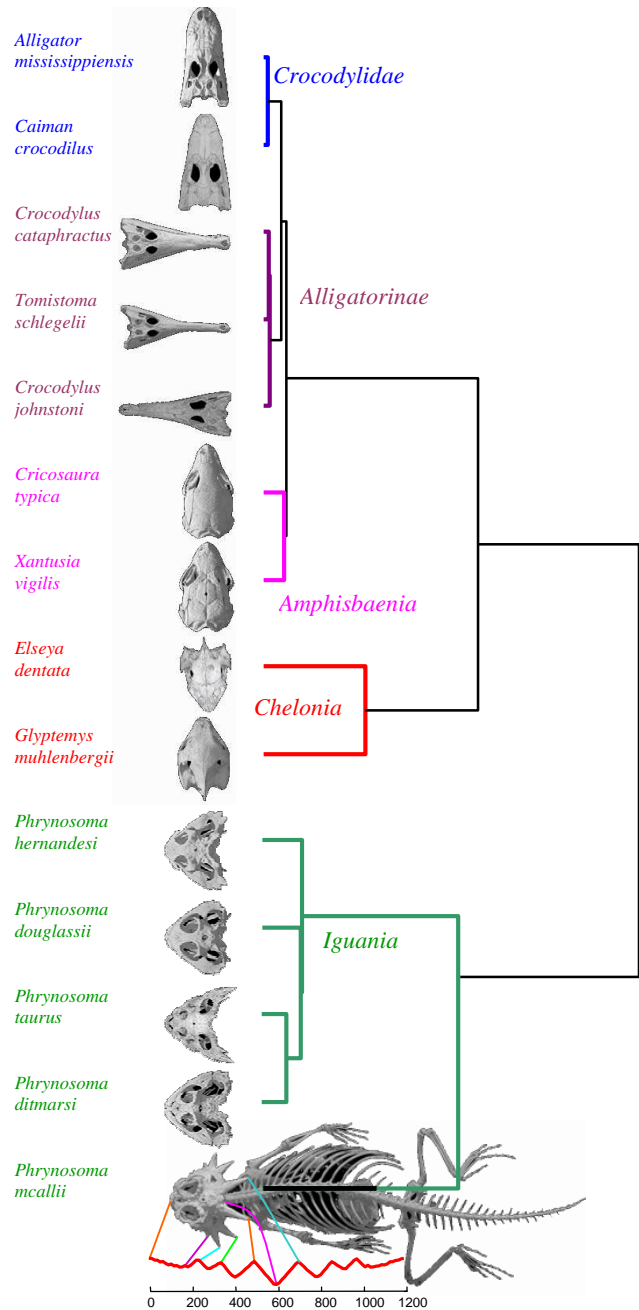


Figure 17: A group average hierarchical clustering of fourteen reptile skulls based on the superior view, using DTW distance

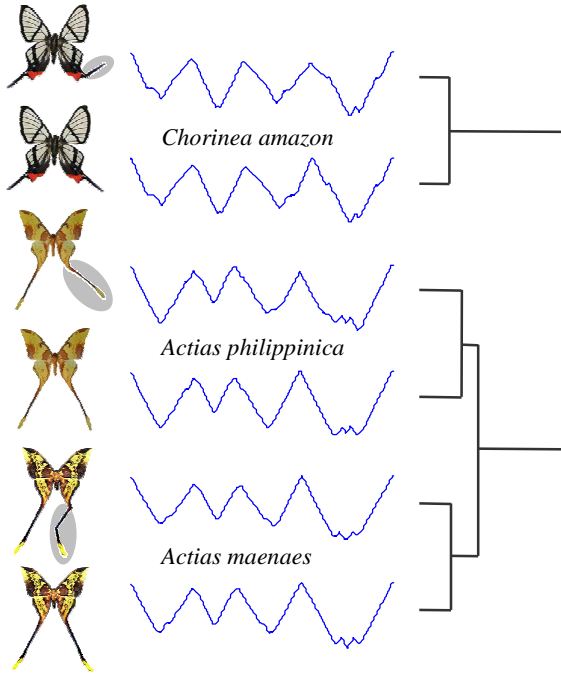


Figure 18: An experiment to demonstrate that the centroid method is reasonably articulation invariant. The gray highlighted areas have been randomly “tweaked” in a photo editing program

As we can see, the one dimensional representation has hardly changed, and the clustering correctly groups the three pairs. We found that using DTW we can even more radically distort the shapes and achieve similar results.

Given the above, why do boundary based methods have such a poor reputation for domains where articulation is a problem [33]? We believe the answer is not intrinsic to boundary based methods, but lies in the measures typically used on them, especially the Hausdorff distance and its many variants. Consider the following thought experiment. Imagine we have two identical shapes; solid automobiles. Assume that they have identical antenna protruding from their roofs. As such, the Hausdorff distance between them is zero, but if we bend the antenna in the spirit of Figure 18, we can trivially increase the Hausdorff distance to one meter.

In addition to the above, the results in Table 8 already hinted at the articulation invariance of our chosen representation. Many of the datasets considered have significant articulation. For example the face dataset considers classes with both closed-lip and laughing/yawning people, the two leaf dataset have significant amounts of articulation at the stem, and the Yoga dataset features very flexible people in version poses.

Finally, we note that paper [25] uses the ideas in the conference version of this work to index hand geometries for biometrics. It is clear that the human hand has a high degree of articulation.

5.3 Main Memory Experiments

There is increasing awareness that comparing two competing approaches using only CPU time opens the possibility of implementation bias [17]. As a simple example, while the Haar wavelet transform is $O(n)$ and DFT is $O(n \log n)$, the DFT is *much* faster in the popular language Matlab, simply because it is a highly optimized subroutine. For this reason many recent papers compare approaches with some implementation-free metric [16][30][37][38]. As we noted earlier, the variable “num_steps”

returned by Table 1 and Table 5 allows an implementation free measure to compare performance.

For Euclidean distance queries we compare to *brute force* and *Fourier* (FFT) methods, which are the only competitors to also guarantee no false dismissals. The cost model for the FFT lower bound is $n \log n$ steps. If the FFT lower bound fails we allow the approach to avail of our early abandoning techniques discussed in Section 3.

We tested on two shape datasets, a homogeneous database of 16,000 projectile point images, all of length 251 and a heterogeneous dataset consisting of all the data used in the classification experiments, plus 1,000 projectile points. In total the heterogeneous dataset contains 5,844 objects of length 1,024. To measure the performance we averaged over 50 runs, with the query object randomly chosen and removed from the dataset.

We measure the average number of steps required by each approach for a single comparison of two shapes, divided by the number of steps require by brute force. For our method, we include a startup cost of $O(n^2)$, which is the time require to build the wedges. Because the utility of early abandoning depends on the value of the best-so-far, we expect our method to do better as we see larger and larger datasets.

Figure 19 shows the results on the projectile points dataset using Euclidean distance.

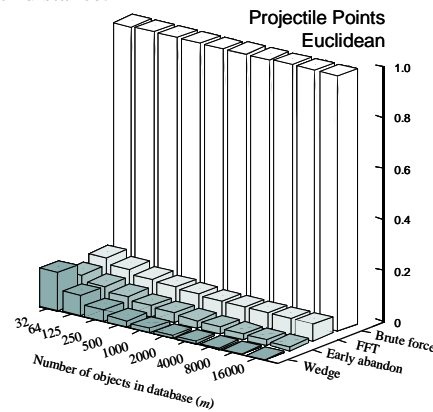


Figure 19: The relative performance of four algorithms on the Projectile Points dataset using the Euclidean distance measure

We can see that for small datasets our approach is slightly worse than *FFT* and simple *Early abandon* because we had to spend some time building the wedges. However, by the time we have seen 64 objects we have already broken even, and thereafter rapidly race towards beating *FFT* and *Early abandon* by one order of magnitude and *Brute force* by two orders of magnitude.

The results on the projectile points dataset using DTW are shown in Figure 20, and are even more dramatic.

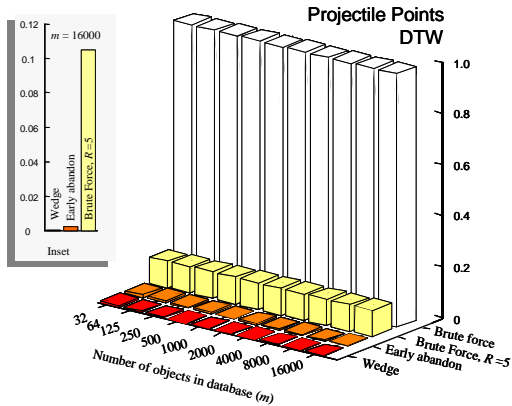


Figure 20: The relative performance of four algorithms on the Projectile Points dataset using the DTW distance measure. The inset shows a zoom-in of the 3 best algorithms when $m = 16,000$

Here the cost of building the wedges is dwarfed by a single brute force DTW-rotation-invariant comparison, so our approach is faster even for a database of size 3. By the time we have examined the entire database, our approach is more than 5,000 times faster than the brute force approach. It is interesting to note that the early abandoning strategy is by itself quite competitive, yet to our knowledge no one uses it. We suspect this is because most people are more familiar with the elegant and terse recursive version of DTW, which does not allow early abandoning, than the iterative implementation, which does. Note however that even though our highly optimized early abandoning strategy is competitive, our wedge approach is still an order of magnitude faster once the dataset is larger than 500 objects.

Sometimes indexing methods that work well for highly homogeneous datasets do not work well for heterogeneous datasets, and vice versa. We consider this possibility by testing on the heterogeneous dataset in Figure 21.

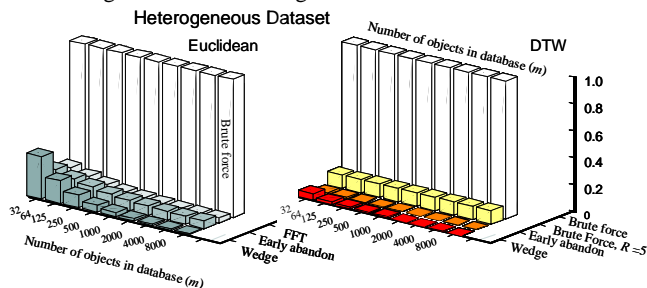


Figure 21: The relative performance of four algorithms on the Heterogeneous dataset using Euclidean distance (left) and DTW (right)

In this dataset it takes our wedge approach slightly longer to beat *Early abandon* (and *FFT* for Euclidean search), however by the time we have seen 8,000 objects our approach is two orders of magnitude faster than its Euclidean competitors, and for DTW it is an order of magnitude faster than *Early abandon* and 3,976 times faster than brute force.

Recall that our algorithm requires the setting of a single parameter, the number of intervals to search for a new value for K every time the *bestSoFar* variable is updated. In all the experiments above this value was set to 5. We found that we can change this value to any number in the range 3 to 20 without affecting the performance of our algorithm by more than 4%, we therefore omit further discussion of this parameter setting.

The Time Series Center at Harvard University Initiative in Innovative Computing has collected light curves from various completed surveys (total 100 million examples) and is collecting data from an on-going survey (TAOS) which is producing few billion additional examples. While light curves have been collected for decades it is only recent years in which we have begun to see serious efforts to index and data mine them. For consistency we only consider the indexing of the small hand labelled set of examples use in the classification experiments in Table 8. Figure 22 shows the performance of the four rival methods on the light curves under the Euclidean distance.

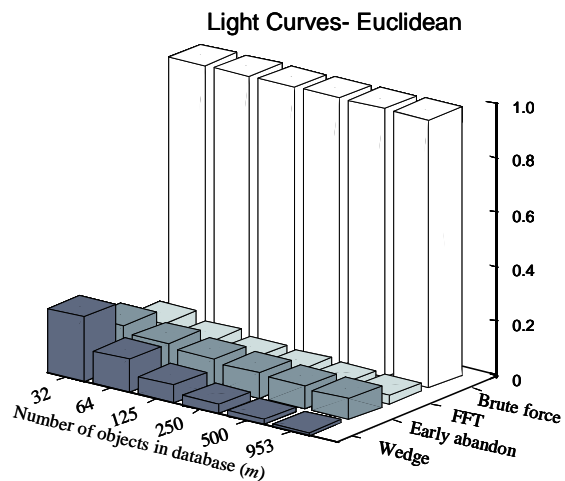


Figure 22: The relative performance of four algorithms on the light curve dataset using Euclidean distance

As before, our approach is slightly slower on small datasets due to the setup overhead. However once the dataset has more than 125 objects the wedge-based approach is slightly faster, and by the time we see the full dataset it is an order of magnitude better than the FFT approach.

Recall that in the classification experiments shown in Table 8, the classification of light curves is significantly faster with the DTW distance. Figure 23 shows the performance of four rival methods on the light curves under the Euclidean distance.

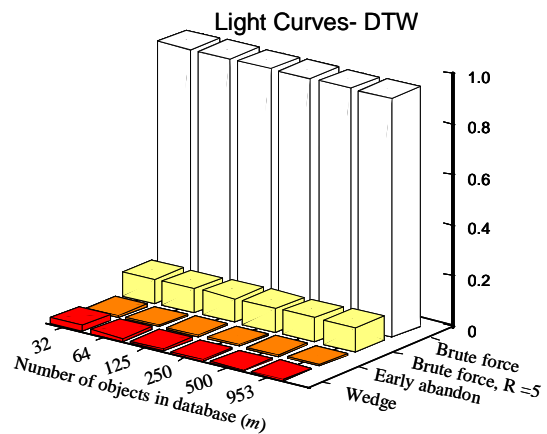


Figure 23: The relative performance of four algorithms on the light curve dataset using DTW distance

As in the shape dataset, our method is several orders of magnitude faster.

As a final sanity check we also measured the wall clock time of our best implementation of all method. The results are essentially identical to those shown above and are omitted for clarity.

5.4 Disk Access Experiments

The results in the previous section show that we can do true rotation invariant matching so fast that CPU time is no longer the bottleneck, and we should therefore also attempt to minimize disk accesses. We will compare to Linear Scan, which is the only other competitor that we are aware of that allows exact rotation invariant indexing under Euclidean distance and DTW with a guarantee of no false dismissals. Recall that the lower bound used by the VP-tree requires transforming the signal to the Fourier space and calculating the Euclidean distance between the coefficient magnitudes [38]. It is well understood that most of the energy of the signal will be concentrated in a relatively small number of these coefficients [37] and that using just a few large valued coefficients is better than using all of them. We therefore will perform experiments keeping just the first D coefficients, where $D = \{4, 8, 16, 32\}$.

We count the fraction of items that must be retrieved from disk. Figure 24 illustrates the results for the full projectile points and heterogeneous datasets over a range of dimensionalities.

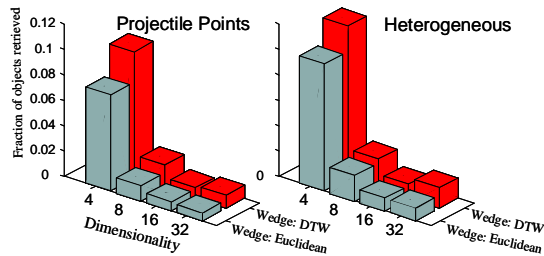


Figure 24: The fraction of items retrieved from disk to answer a 1-nearest neighbor query, using dimensionalities $D = \{4, 8, 16, 32\}$.

6. CONCLUSIONS AND FUTURE WORK

We have introduced a method to support fast rotation-invariant search of large shape datasets with arbitrary representations and distance functions. Our method supports rotation limited queries and mirror image invariance *if desired*.

Future work includes both extensions and applications of the current work. We will attempt to extend this approach to the indexing of 3D shapes, and we have begun to use our algorithm as a subroutine in several data mining algorithms which attempt to cluster, classify and discover motifs in a variety of anthropological datasets, including petroglyph and projectile point databases.

Reproducible Research Statement: All datasets and images used in this work are freely available at this URL [14].

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