Faster Retrieval with a Two-Pass Dynamic-Time-Warping Lower Bound

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Abstract

The Dynamic Time Warping (DTW) is a popular similarity measure between time series. The DTW fails to satisfy the triangle inequality and its computation requires quadratic time. Hence, to find closest neighbors quickly, we use bounding techniques. We can avoid most DTW computations with an inexpensive lower bound (LB_{Keogh}). We compare LB_{Keogh} with a tighter lower bound (LB_{Improved}). We find that LB_{Improved}-based search is faster. As an example, our approach is 2–3 times faster over random-walk and shape time series.

Key words: time series, very large databases, indexing, classification

1 Introduction

Dynamic Time Warping (DTW) was initially introduced to recognize spoken words [1], but it has since been applied to a wide range of information retrieval and database problems: handwriting recognition [2,3], signature recognition [4,5], image de-interlacing [6], appearance matching for security purposes [7], whale vocalization classification [8], query by humming [9,10], classification of motor activities [11], face localization [12], chromosome classification [13], shape retrieval [14,15], and so on. Unlike the Euclidean distance, DTW optimally aligns or “warp” the data points of two time series (see Fig. 1).

When the distance between two time series forms a metric, such as the Euclidean distance or the Hamming distance, several indexing or search tech-
niques have been proposed [16–20]. However, even assuming that we have a metric, Weber et al. have shown that the performance of any indexing scheme degrades to that of a sequential scan, when there are more than a few dimensions [21]. Otherwise—when the distance is not a metric or that the number of dimensions is too large—we use bounding techniques such as the Generic multimedia object indexing (GEMINI) [22]. We quickly discard (most) false positives by computing a lower bound.

Fig. 1. Dynamic Time Warping example

Ratanamahatana and Keogh [23] argue that their lower bound (LB Keogh) cannot be improved upon. To make their point, they report that LB Keogh allows them to prune out over 90% of all DTW computations on several data sets.

We are able to improve upon LB Keogh as follows. The first step of our two-pass approach is LB Keogh itself. If this first lower bound is sufficient to discard the candidate, then the computation terminates and the next candidate is considered. Otherwise, we process the time series a second time to increase the lower bound (see Fig. 5). If this second lower bound is large enough, the candidate is pruned, otherwise we compute the full DTW. We show experimentally that the two-pass approach can be several times faster.

The paper is organized as follows. In Section 4, we define the DTW in a generic manner as the minimization of the \( l_p \) norm (\( DTW_p \)). Among other things, we show that if \( x \) and \( y \) are separated by a constant \( (x \geq c \geq y \) or \( x \leq c \leq y \) then the \( DTW_1 \) is the \( l_1 \) norm (see Proposition 1). In Section 5, we compute generic lower bounds on the DTW and their approximation errors using warping envelopes. In Section 6, we show how to compute the warping envelopes quickly. The next two sections introduce LB Keogh and LB Improved respectively. Section 9 presents the application of these lower bounds for multidimensional indexing whereas the last section presents an experimental comparison.
2 Conventions

Time series are arrays of values measured at certain times. For simplicity, we assume a regular sampling rate so that time series are generic arrays of floating-point values. Time series have length $n$ and are indexed from 1 to $n$. The $l_p$ norm of $x$ is $\|x\|_p = (\sum_i |x_i|^p)^{1/p}$ for any integer $0 < p < \infty$ and $\|x\|_\infty = \max_i |x_i|$. The $l_p$ distance between $x$ and $y$ is $\|x - y\|_p$ and it satisfies the triangle inequality $\|x - z\|_p \leq \|x - y\|_p + \|y - z\|_p$ for $1 \leq p \leq \infty$. The distance between a point $x$ and a set or region $S$ is $d(x, S) = \min_{y \in S} d(x, y)$. Other conventions are summarized in Table 1.

| Convention | Description |
|------------|-------------|
| $n$        | length of a time series |
| $\|x\|_p$  | $l_p$ norm |
| DTW$_p$    | monotonic DTW |
| NDTW$_p$   | non-monotonic DTW |
| $w$        | DTW locality constraint |
| $U(x), L(x)$ | warping envelope (see Section 5) |
| $H(x, y)$  | projection of $x$ on $y$ (see Equation 1) |

3 Related Works

Beside DTW, several similarity metrics have been proposed including the directed and general Hausdorff distance, Pearson’s correlation, nonlinear elastic matching distance [24], Edit distance with Real Penalty (ERP) [25], Needleman-Wunsch similarity [26], Smith-Waterman similarity [27], and SimilB [28].

Boundary-based lower-bound functions sometimes outperform LB_Keogh [29].

We can also quantize [30] the time series.

Sakurai et al. [31] have shown that retrieval under the DTW can be faster by mixing progressively finer resolution and by applying early abandoning [32] to the dynamic programming computation.
4 Dynamic Time Warping

A many-to-many matching between the data points in time series $x$ and the data point in time series $y$ matches every data point $x_i$ in $x$ with at least one data point $y_j$ in $y$, and every data point in $y$ with at least a data point in $x$. The set of matches $(i, j)$ forms a warping path $\Gamma$. We define the DTW as the minimization of the $l_p$ norm of the differences $\{x_i - y_j\}_{(i,j)\in \Gamma}$ over all warping paths. A warping path is minimal if there is no subset $\Gamma'$ of $\Gamma$ forming an warping path: for simplicity we require all warping paths to be minimal.

In computing the DTW distance, we commonly require the warping to remain local. For time series $x$ and $y$, we align values $x_i$ and $y_j$ only if $|i - j| \leq w$ for some locality constraint $w \geq 0$ [1]. When $w = 0$, the DTW becomes the $l_p$ distance whereas when $w \geq n$, the DTW has no locality constraint. The value of the DTW diminishes monotonically as $w$ increases. (We do not consider other forms of locality constraints such as the Itakura parallelogram [33].)

Other than locality, DTW can be monotonic: if we align value $x_i$ with value $y_j$, then we cannot align value $x_{i+1}$ with a value appearing before $y_j$ ($y_{j'}$ for $j' < j$).

We note the DTW distance between $x$ and $y$ using the $l_p$ norm as $\text{DTW}_p(x, y)$ when it is monotonic and as $\text{NDTW}_p(x, y)$ when monotonicity is not required.

By dynamic programming, the monotonic DTW requires $O(wn)$ time. A typical value of $w$ is $n/10$ [23] so that the DTW is in $O(n^2)$. To compute the DTW, we use the following recursive formula. Given an array $x$, we write the suffix starting at position $i$, $x_{(i)} = x_i, x_{i+1}, \ldots, x_n$. The symbol $\oplus$ is the exclusive or. Write $q_{i,j} = \text{DTW}_p(x_{(i)}, y_{(j)})^p$ so that $\text{DTW}_p(x, y) = \sqrt[p]{q_{1,1}}$, then

$$q_{i,j} = \begin{cases} 0 & \text{if } |x_{(i)}| = |y_{(j)}| = 0 \\
\infty & \text{if } |x_{(i)}| = 0 \oplus |y_{(j)}| = 0 \\
|x_i - y_j|^p + \min\{q_{i+1,j}, q_{i,j+1}, q_{i+1,j+1}\} & \text{otherwise.}
\end{cases}$$

For $p = \infty$, we rewrite the preceding recursive formula with $q_{i,j} = \text{DTW}_\infty(x_{(i)}, y_{(j)})$, and $q_{i,j} = \max(|x_i - y_j|, \min\{q_{i+1,j}, q_{i,j+1}, q_{i+1,j+1}\})$ when $|x_{(i)}| \neq 0$, $|y_{(j)}| \neq 0$, and $|i - j| \leq w$.

We can compute $\text{NDTW}_1$ without locality constraint in $O(n \log n)$ [34]: if the values of the time series are already sorted, the computation is in $O(n)$ time.

We can express the solution of the DTW problem as an alignment of the two
initial time series (such as \(x = 0,1,1,0\) and \(y = 0,1,0,0\)) where some of the values are repeated (such as \(x' = 0,1,1,0,0\) and \(y' = 0,1,1,0,0\)). If we allow non-monotonicity (NDTW), then values can also be inverted.

The non-monotonic DTW is no larger than the monotonic DTW which is itself no larger than the \(l_p\) norm: \(\text{NDTW}_p(x,y) \leq \text{DTW}_p(x,y) \leq \|x-y\|_p\) for all \(0 < p \leq \infty\).

The DTW has the property that if the time series are value-separated, then the DTW is the \(l_1\) norm as the next proposition shows. In Figs. 3 and 4, we present value-separated functions: their DTW is the area between the curves.

**Proposition 1** If \(x\) and \(y\) are such that either \(x \geq c \geq y\) or \(x \leq c \leq y\) for some constant \(c\), then \(\text{DTW}_1(x,y) = \text{NDTW}_1(x,y) = \|x-y\|_1\).

**PROOF.** Assume \(x \geq c \geq y\). Consider the two aligned (and extended) time series \(x', y'\) such that \(\text{NDTW}_1(x,y) = \|x' - y'\|_1\). We have that \(x' \geq c \geq y'\) and \(\text{NDTW}_1(x,y) = \|x' - y'\|_1 = \sum_i |x'_i - y'_i| = \sum_i |x'_i - c| + |c - y'_i| = \|x' - c\|_1 + \|c - y'\|_1 \geq \|x - c\|_1 + \|c - y\|_1 = \|x - y\|_1\). Since we also have \(\text{NDTW}_1(x,y) \leq \text{DTW}_1(x,y) \leq \|x-y\|_1\), the equality follows.

Proposition 1 does not hold for \(p > 1\): \(\text{DTW}_2((0,0,1,0),(2,3,2,2)) = \sqrt{17}\) whereas \(\|(0,0,1,0) - (2,3,2,2)\|_2 = \sqrt{18}\).

### 5 Computing Lower Bounds on the DTW

Given a time series \(x\), define \(U(x)_i = \max_k \{x_k||k-i| \leq w\}\) and \(L(x)_i = \min_k \{x_k||k-i| \leq w\}\) for \(i = 1, \ldots, n\). The pair \(U(x)\) and \(L(x)\) forms the warping envelope of \(x\) (see Fig. 2). We leave the locality constraint \(w\) implicit.

The theorem of this section has an elementary proof requiring only the following technical lemma.

**Lemma 1** If \(b \in [a,c]\) then \((c-a)^p \geq (c-b)^p + (b-a)^p\) for \(1 \leq p < \infty\).

**PROOF.** For \(p = 1\), \((c-b)^p + (b-a)^p = (c-a)^p\). For \(p > 1\), by deriving \((c-b)^p + (b-a)^p\) with respect to \(b\), we can show that it is minimized when \(b = (c+a)/2\) and maximized when \(b \in \{a,c\}\). The maximal value is \((c-a)^p\). Hence the result.
The following theorem introduces a generic result that we use to derive two lower bounds for the DTW including the original Keogh-Ratanamahatana result [35]. Indeed, this new result not only implies the lower bound $LB_{Keogh}$, but it also provides a lower bound to the error made by $LB_{Keogh}$, thus allowing a tighter lower bound ($LB_{Improved}$).

**Theorem 1** Given two equal-length time series $x$ and $y$ and $1 \leq p < \infty$, then for any time series $h$ satisfying $x_i \geq h_i \geq U(y)_i$ or $x_i \leq h_i \leq L(y)_i$ or $h_i = x_i$ for all indexes $i$, we have

$$DTW_p(x, y)^p \geq NDTW_p(x, y)^p \geq \|x - h\|_p^p + NDTW_p(h, y)^p.$$ 

For $p = \infty$, a similar result is true: $DTW_\infty(x, y) \geq NDTW_\infty(x, y) \geq \max(\|x - h\|_\infty, NDTW_\infty(h, y))$.

**Proof.** Suppose that $1 \leq p < \infty$. Let $\Gamma$ be a warping path such that $NDTW_p(x, y)_p = \sum_{(i,j) \in \Gamma} |x_i - y_j|^p$. By the constraint on $h$ and Lemma 1, we have that $|x_i - y_j|^p \geq |x_i - h_i|^p + |h_i - y_j|^p$ for any $(i, j) \in \Gamma$ since $h_i \in [\min(x_i, y_j), \max(x_i, y_j)]$. Hence, we have that $NDTW_p(x, y)^p \geq \sum_{(i,j) \in \Gamma} |x_i - h_i|^p + |h_i - y_j|^p \geq \|x - h\|_p^p + \sum_{(i,j) \in \Gamma} |h_i - y_j|^p$. This proves the result since $\sum_{(i,j) \in \Gamma} |h_i - y_j| \geq NDTW_p(h, y)$. For $p = \infty$, we have that

$$NDTW_\infty(x, y) = \max_{(i,j) \in \Gamma} |x_i - y_j| \leq \max_{(i,j) \in \Gamma} \max(|x_i - h_i|, |h_i - y_j|)$$

$$= \max(\|x - h\|_\infty, NDTW_\infty(h, y)),$$

concluding the proof.
While Theorem 1 defines a lower bound ($\|x-h\|_p$), the next proposition shows that this lower bound must be a tight approximation as long as $h$ is close to $y$ in the $l_p$ norm.

**Proposition 2** Given two equal-length time series $x$ and $y$, and $1 \leq p \leq \infty$ with $h$ as in Theorem 1, we have that $\|x-h\|_p$ approximates both $DTW_p(x,y)$ and $NDTW_p(x,y)$ within $\|h-y\|_p$.

**Proof.** By the triangle inequality over $l_p$, we have $\|x-h\|_p + \|h-y\|_p \geq \|x-y\|_p$. Since $\|x-y\|_p \geq DTW_p(x,y)$, we have $\|x-h\|_p + \|h-y\|_p \geq DTW_p(x,y)$, and hence $\|h-y\|_p \geq DTW_p(x,y) - \|x-h\|_p$. This proves the result since by Theorem 1, we have that $DTW_p(x,y) \geq NDTW_p(x,y) \geq \|x-h\|_p$.

This bound on the approximation error is reasonably tight. If $x$ and $y$ are separated by a constant, then $DTW_1(x,y) = \|x-y\|_1$ by Proposition 1 and $\|x-y\|_1 = \sum_i |x_i - y_i| = \sum_i |x_i - h_i| + |h_i - y_i| = \|x-h\|_1 + \|h-y\|_1$. Hence, the approximation error is exactly $\|h-y\|_1$ in such instances.

6 Warping Envelopes

The computation of the warping envelope $U(x), L(x)$ requires $O(nw)$ time using the naive approach of repeatedly computing the maximum and the minimum over windows. Instead, we compute the envelope with at most $3n$ comparisons between data-point values [36] using Algorithm 1.

7 LB_Keogh

Let $H(x,y)$ be the projection of $x$ on $y$ defined as

$$H(x,y)_i = \begin{cases} U(y)_i & \text{if } x_i \geq U(y)_i \\ L(y)_i & \text{if } x_i \leq L(y)_i \\ x_i & \text{otherwise,} \end{cases}$$

for $i = 1, 2, \ldots, n$. We have that $H(x,y)$ is in the envelope of $y$. By Theorem 1 and setting $h = H(x,y)$, we have that $NDTW_p(x,y)^p \geq \|x-H(x,y)\|_p^p$ and $NDTW_p(H(x,y),y)^p$ for $1 \leq p < \infty$. Write $LB_{Keogh}(x,y) = \|x-H(x,y)\|_p$ (see Fig. 3), then $LB_{Keogh}(x,y)$ is a lower bound to $NDTW_p(x,y)$ and thus $DTW_p(x,y)$. The following corollary follows from Theorem 1 and Proposition 2.
Algorithm 1 Streaming algorithm to compute the warping envelope using no more than $3n$ comparisons

- **input** a time series $y$ indexed from 1 to $n$
- **input** some DTW locality constraint $w$
- **return** warping envelope $U, L$ (two time series of length $n$)

1. $u, l \leftarrow$ empty double-ended queues, we append to “back”
2. append 1 to $u$

3. for $i$ in $\{2, \ldots, n\}$ do
   4. if $i \geq w + 1$ then
      5. $U_{i-w} \leftarrow y_{\text{front}(u)}, L_{i-w} \leftarrow y_{\text{front}(l)}$
      6. if $y_i > y_{i-1}$ then
         7. pop $u$ from back
         8. while $y_i > y_{\text{back}(u)}$ do
            9. pop $u$ from back
      10. else
          11. pop $l$ from back
          12. while $y_i < y_{\text{back}(l)}$ do
             13. pop $l$ from back
   14. append $i$ to $u$ and $l$

15. if $i = 2w + 1 + \text{front}(u)$ then
   16. pop $u$ from front
17. else if $i = 2w + 1 + \text{front}(l)$ then
   18. pop $l$ from front

19. for $i$ in $\{n+1, \ldots, n+w\}$ do
   20. $U_{i-w} \leftarrow y_{\text{front}(u)}, L_{i-w} \leftarrow y_{\text{front}(l)}$
   21. if $i-\text{front}(u) \geq 2w + 1$ then
      22. pop $u$ from front
   23. if $i-\text{front}(l) \geq 2w + 1$ then
      24. pop $l$ from front

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Fig. 3. LB Keogh example: the area of the marked region is $\text{LB}_\text{Keogh}_1(x, y)$
Corollary 1 Given two equal-length time series $x$ and $y$ and $1 \leq p \leq \infty$, then

- $LB_{\text{Keogh}}(x, y)$ is a lower bound to the DTW:
  \[ DTW_p(x, y) \geq NDTW_p(x, y) \geq LB_{\text{Keogh}}(x, y); \]

- the accuracy of $LB_{\text{Keogh}}$ is bounded by the distance to the envelope:
  \[ DTW_p(x, y) - LB_{\text{Keogh}}(x, y) \leq \|\max\{U(y)_i - y_i, y_i - L(y)_i\}_i\|_p \]
  for all $x$.

Algorithm 2 shows how $LB_{\text{Keogh}}$ can be used to find a nearest neighbor in a time series database. We used DTW$_1$ for all implementations (see Appendix C). The computation of the envelope of the query time series is done once (see line 4). The lower bound is computed in lines 7 to 12. If the lower bound is sufficiently large, the DTW is not computed (see line 13). Ignoring the computation of the full DTW, at most $(2N + 3)n$ comparisons between data points are required to process a database containing $N$ time series.

**Algorithm 2** $LB_{\text{Keogh}}$-based Nearest-Neighbor algorithm

1: input a time series $y$ indexed from 1 to $n$
2: input a set $S$ of candidate time series
3: return the nearest neighbor $B$ to $y$ in $S$ under DTW$_1$
4: $U, L \leftarrow$ envelope($y$)
5: $b \leftarrow \infty$ \{$b$ stores $\min_{x \in S} \text{DTW}_1(x, y)$\}
6: for candidate $x$ in $S$ do
7: \hspace{1em} $\beta \leftarrow 0$ \{$\beta$ stores the lower bound\}
8: \hspace{1em} for $i \in \{1, 2, \ldots, n\}$ do
9: \hspace{2em} if $x_i > U_i$ then
10: \hspace{3em} $\beta \leftarrow \beta + x_i - U_i$
11: \hspace{2em} else if $x_i < L_i$ then
12: \hspace{3em} $\beta \leftarrow \beta + L_i - x_i$
13: \hspace{2em} if $\beta < b$ then
14: \hspace{3em} $t \leftarrow \text{DTW}_1(a, c)$ \{We compute the full DTW.\}
15: \hspace{2em} if $t < b$ then
16: \hspace{3em} $b \leftarrow t$
17: \hspace{2em} $B \leftarrow c$

8 $LB_{\text{Improved}}$

In the previous Section, we saw that $NDTW_p(x, y)^p \geq LB_{\text{Keogh}}(x, y)^p + NDTW_p(H(x, y), y)^p$ for $1 \leq p \leq \infty$. In turn, we have $NDTW_p(H(x, y), y)$ ≥
LB_Improved

Fig. 4. LB_Improved example: the area of the marked region is LB_Improved(x, y) for 1 ≤ p < ∞. By definition, we have LB_Improved_p(x, y) ≥ LB_Keogh_p(x, y).

Corollary 2 Given two equal-length time series x and y and 1 ≤ p < ∞, then LB_Improved_p(x, y) is a lower bound to the DTW: DTW_p(x, y) ≥ NDTW_p(x, y) ≥ LB_Improved_p(x, y).

PROOF. Recall that LB_Keogh_p(x, y) = \|x - H(x, y)\|_p. First apply Theorem 1: DTW_p(x, y)^p ≥ NDTW_p(x, y)^p ≥ LB_Keogh_p(x, y)^p + NDTW_p(H(x, y), y)^p. Apply Theorem 1 once more: NDTW_p(H(x, y), y)^p ≥ LB_Keogh_p(y, H(x, y))^p. By substitution, we get DTW_p(x, y)^p ≥ NDTW_p(x, y)^p ≥ LB_Keogh_p(x, y)^p + LB_Keogh_p(y, H(x, y))^p thus proving the result.

Algorithm 3 shows how to apply LB_Improved as a two-step process (see Fig. 5). Initially, for each candidate x, we compute the lower bound LB_Keogh_1(x, y) (see lines 8 to 15). If this lower bound is sufficiently large, the candidate is discarded (see line 16), otherwise we add LB_Keogh_1(y, H(x, y)) to LB_Keogh_1(x, y), in effect computing LB_Improved_1(x, y) (see lines 17 to 22). If this larger lower bound is sufficiently large, the candidate is finally discarded (see line 23). Otherwise, we compute the full DTW. If α is the fraction of candidates pruned by
LB_Keogh, at most \((2N+3)n + 5(1-\alpha)Nn\) comparisons between data points are required to process a database containing \(N\) time series.

**Algorithm 3** LB_Improved-based Nearest-Neighbor algorithm

1: **input** a time series \(y\) indexed from 1 to \(n\)
2: **input** a set \(S\) of candidate time series
3: **return** the nearest neighbor \(B\) to \(y\) in \(S\) under DTW
4: \(U, L \leftarrow \text{envelope}(y)\)
5: \(b \leftarrow \infty\) \{\(b\) stores \(\min_{x \in S} \text{DTW}_1(x, y)\)\}
6: **for** candidate \(x\) in \(S\) **do**
7: copy \(x\) to \(x'\) \{\(x'\) will store the projection of \(x\) on \(y\)\}
8: \(\beta \leftarrow 0\) \{\(\beta\) stores the lower bound\}
9: **for** \(i \in \{1, 2, \ldots, n\}\) **do**
10: **if** \(x_i > U_i\) **then**
11: \(\beta \leftarrow \beta + x_i - U_i\)
12: \(x'_i = U_i\)
13: **else if** \(x_i < L_i\) **then**
14: \(\beta \leftarrow \beta + L_i - x_i\)
15: \(x'_i = L_i\)
16: **if** \(\beta < b\) **then**
17: \(U', L' \leftarrow \text{envelope}(x')\)
18: **for** \(i \in \{1, 2, \ldots, n\}\) **do**
19: **if** \(y_i > U'_i\) **then**
20: \(\beta \leftarrow \beta + y_i - U'_i\)
21: **else if** \(y_i < L'_i\) **then**
22: \(\beta \leftarrow \beta + L'_i - y_i\)
23: **if** \(\beta < b\) **then**
24: \(t \leftarrow \text{DTW}_1(a, c)\) \{We compute the full DTW.\}
25: **if** \(t < b\) **then**
26: \(b \leftarrow t\)
27: \(B \leftarrow c\)

9 Using a multidimensional indexing structure

The running time of Algorithms 2 and 3 may be improved if we use a multidimensional index such as an R*-tree [37]. Unfortunately, the performance of such an index diminishes quickly as the number of dimensions increases [21]. To solve this problem, several dimensionality reduction techniques are possible such as piecewise linear [38–40] segmentation. Following Zhu and Shasha [10], we project time series and their envelopes on a \(d\)-dimensional space using piecewise sums: \(P_d(x) = (\sum_{i \in C_j} x_i)_j\) where \(C_1, C_2, \ldots, C_d\) is a disjoint cover of \(\{1, 2, \ldots, n\}\). Unlike Zhu and Shasha, we do not require the intervals to have equal length. The \(l_1\) distance between \(P_d(y)\) and the minimum bounding hyperrectangle containing \(P_d(L(x))\) and \(P_d(U(x))\) is a lower bound to the
We begin with $y$ and its envelope $L(y), U(y)$.

We compare candidate $x$ with the envelope $L(y), U(y)$.

The difference is $\text{LB}_{\text{Keogh}}(x, y)$.

We compute $x'$, the projection of $x$ on the envelope $L(y), U(y)$.

We compute the envelope of $x'$.

The difference between $y$ and the envelope $L(x'), U(x')$ is added to $\text{LB}_{\text{Keogh}}$ to compute $\text{LB}_{\text{Improved}}$.

Fig. 5. Computation of $\text{LB}_{\text{Improved}}$ as in Algorithm 3

\[ \text{DTW}_1(x, y) : \]

\[ \text{DTW}_1(x, y) \geq \text{LB}_{\text{Keogh}}_1(x, y) \]

\[ = \sum_{i=1}^{n} d(x_i, [L(y)_i, U(y)_i]) \]

\[ \geq \sum_{j=1}^{d} d(P_d(x)_j, [P_d(L(y))_j, P_d(U(y))_j]). \]
For our experiments, we chose the cover \( C_j = \lfloor 1 + (j - 1)\frac{n}{d} \rfloor, j\lfloor \frac{n}{d} \rfloor \) for \( j = 1, \ldots, d - 1 \) and \( C_d = \lfloor 1 + (d - 1)\frac{n}{d} \rfloor, n \).

We can summarize the Zhu-Shasha R*-tree algorithm as follows:

1. for each time series \( x \) in the database, add \( P_d(x) \) to the R*-tree;
2. given a query time series \( y \), compute its envelope \( E = P_d(L(y)), P_d(U(y)) \);
3. starting with \( b = \infty \), iterate over all candidate \( P_d(x) \) at a \( l_1 \) distance \( b \) from the envelope \( E \) using the R*-tree, once a candidate is found, update \( b \) with DTW\(_1\)(\( x, y \)) and repeat until you have exhausted all candidates.

This algorithm is correct because the distance between \( E \) and \( P_d(x) \) is a lower bound to DTW\(_1\)(\( x, y \)). However, dimensionality reduction diminishes the pruning power of LB\(_{Keogh}\) : \( d(E, P_d(x)) \leq \text{LB}_{\text{Keogh}}(x, y) \). Hence, we propose a new algorithm (R*-TREE+LB\(_{KEOGH}\)) where instead of immediately updating \( b \) with DTW\(_1\)(\( x, y \)), we first compute the LB\(_{Keogh}\) lower bound between \( x \) and \( y \). Only when it is less than \( b \), do we compute the full DTW. Finally, as a third algorithm (R*-TREE+LB\(_{IMPROVED}\)), we first compute LB\(_{Keogh}\), and if it is less than \( b \), then we compute LB\(_{Improved}\), and only when it is also lower than \( b \) do we compute the DTW, as in Algorithm 3. R*-TREE+LB\(_{IMPROVED}\) has maximal pruning power, whereas Zhu-Shasha R*-tree has the lesser pruning power of the three alternatives.

10 Comparing Zhu-Shasha R*-tree, LB\(_{Keogh}\), and LB\(_{Improved}\)

In this section, we benchmark algorithms Zhu-Shasha R*-tree, R*-TREE+LB\(_{KEOGH}\), and R*-TREE+LB\(_{IMPROVED}\). We know that the LB\(_{Improved}\) approach has at least the pruning power of the other methods, but does more pruning translate into a faster nearest-neighbor retrieval under the DTW distance?

We implemented the algorithms in C++ using an external-memory R*-tree. The time series are stored on disk in a binary flat file. We used the GNU GCC 4.0.2 compiler on an Apple Mac Pro, having two Intel Xeon dual-core processors running at 2.66 GHz with 2 GiB of RAM. No thrashing was observed. We measured the wall-clock total time. In all experiments, we benchmark nearest-neighbor retrieval under the DTW\(_1\). By default, the locality constraint \( w \) is set at 10% \( (w = n/10) \). To ensure reproducibility, our source code is freely available [41], including the script used to generate synthetic data sets. We compute the full DTW using a \( O(nw) \)-time dynamic programming algorithm.

The R*-tree was implemented using the Spatial Index library [42]. In informal
tests, we found that a projection on an 8-dimensional space, as described by Zhu and Shasha, gave good results: substantially larger ($d > 10$) or smaller ($d < 6$) settings gave poorer performance. We used a 4,096-byte page size and a 10-entry internal memory buffer.

For R*-tree+ LB Keogh and R*-tree+LB Improved, we experimented with early abandoning [32] to cancel the computation of the lower bound as soon as the error is too large. While it often improved retrieval time slightly for both LB Keogh and LB Improved, the difference was always small (less than $\approx 1\%$). One explanation is that the candidates produced by the Zhu-Shasha R*-tree are rarely poor enough to warrant efficient early abandoning.

We do not report our benchmarking results over the simple Algorithms 2 and 3. In almost all cases, the R*-tree equivalent—R*-tree+ LB Keogh or R*-tree+LB Improved—was at least slightly better and sometimes several times faster.

10.1 Synthetic data sets

We tested our algorithms using the Cylinder-Bell-Funnel [43] and Control Charts [44] data sets, as well as over two databases of random walks. We generated 256-sample and 1,000-sample random-walk time series using the formula $x_i = x_{i-1} + N(0, 1)$ and $x_1 = 0$.

For each data set, we generated a database of 50,000 time series by adding randomly chosen items. Figs. 6, 7, 8 and 9 show the average timings and pruning ratio averaged over 20 queries based on randomly chosen time series as we consider larger and large fraction of the database. LB Improved prunes between 2 and 4 times more candidates than LB Keogh. R*-tree+LB Improved is faster than Zhu-Shasha R*-tree by a factor between 0 and 6.

We saw almost no performance gain over Zhu-Shasha R*-tree with simple time series such as the Cylinder-Bell-Funnel or the Control Charts data sets. However, in these cases, even LB Improved has modest pruning powers of 40% and 15%. Low pruning means that the computational cost is dominated by the cost of the full DTW.

10.2 Shape data sets

We also considered a large collection of time-series derived from shapes [45,46]. The first data set is made of heterogeneous shapes which resulted in 5,844 1,024-sample times series. The second data set is an arrow-head data set
with of 15 000 251-sample time series. We extracted 50 time series from each data set, and we present the average nearest-neighbor retrieval times and pruning power as we consider various fractions of each database (see Figs. 10 and 11). The results are similar: LB_Improved has twice the pruning power than LB_Keogh, R*-Tree+LB_Improved is twice as fast as R*-Tree+LB_Keogh and over 3 times faster than the Zhu-Shasha R*-tree.
10.3 Locality constraint

The locality constraint has an effect on retrieval times: a large value of $w$ makes the problem more difficult and reduces the pruning power of all methods. In Figs. 12 and 13, we present the retrieval times for $w = 5\%$ and $w = 20\%$. The benefits of $R^*\text{-TREE} + \text{LB\_IMPROVED}$ remain though they are less significant for small locality constraints. Nevertheless, even in this case, $R^*$-
Fig. 12. Average Nearest-Neighbor Retrieval Time for the 256-sample random-walk data set

Fig. 13. Average Nearest-Neighbor Retrieval Time for the arrow-head shape data set

tree+LB_Improved can still be three times faster than Zhu-Shasha R*-tree. For all our data sets and for all values of \( w \in \{5\%, 10\%, 20\%\} \), R*-tree+LB_Improved was always at least as fast as the Zhu-Shasha R*-tree algorithm alone.

11 Conclusion

We have shown that a two-pass pruning technique can improve the retrieval speed by three times or more in several time-series databases. In our implementation, LB_Improved required slightly more computation than LB_Keogh, but its added pruning power was enough to make the overall computation several times faster. Moreover, we showed that pruning candidates left from the Zhu-Shasha R*-tree with the full LB_Keogh alone—without dimensionality reduction—was enough to significantly boost the speed and pruning power. On some synthetic data sets, neither LB_Keogh nor LB_Improved were able to prune enough candidates, making all algorithms comparable in speed.
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A Some Properties of Dynamic Time Warping

The DTW distance can be counterintuitive. As an example, if $x, y, z$ are three time series such that $x \leq y \leq z$ pointwise, then it does not follow that
Lemma 2 For any $y$ or $x$, the DTW becomes the $l_p$ distance when either $x$ or $y$ is constant.

The warping path aligns $x_i$ from time series $x$ and $y_j$ from time series $y$ if $(i, j) \in \Gamma$. The next proposition is a general constraint on warping paths.

Proposition 3 Consider any two time series $x$ and $y$. For any minimal warping path, if $x_i$ is aligned with $y_j$, then either $x_i$ is aligned only with $y_j$ or $y_j$ is aligned only with $x_i$. Therefore the length of a minimal warping path is at most $2n - 2$ when $n > 1$.

Proof. Suppose that the result is not true. Then there is $x_k, x_i$ and $y_l, y_j$ such that $x_k$ and $x_i$ are aligned with $y_j$, and $y_l$ and $y_j$ are aligned with $x_i$. We can delete $(k, j)$ from the warping path and still have a warping path. A contradiction.

Next, we show that warping path is no longer than $2n - 2$. Let $n_1$ be the number of points in $x$ aligned with only one point in $y$, and let $n_2$ be the number of points in $y$ aligned with only one point in $x$. The cardinality of a minimal warping path is bounded by $n_1 + n_2$. If $n_1 = n$ or $n_2 = n$, then $n_1 = n_2 = n$ and the warping path has cardinality $n$ which is no larger than $2n - 2$ for $n > 1$. Otherwise, $n_1 \leq n - 1$ and $n_2 \leq n - 1$, and $n_1 + n_2 < 2n - 2$.

The next lemma shows that the DTW becomes the $l_p$ distance when either $x$ or $y$ is constant.

Lemma 2 For any $0 < p \leq \infty$, if $y = c$ is a constant, then $NDTW_p(x, y) = DTW_p(x, y) = \|x - y\|_p$.

When $p = \infty$, a stronger result is true: if $y = x + c$ for some constant $c$, then $NDTW_\infty(x, y) = DTW_\infty(x, y) = \|x - y\|_\infty$. Indeed, $NDTW_\infty(x, y) \geq |\max(y) - \max(x)| = c = \|x - y\|_\infty \geq \|x - y\|_\infty$ which shows the result. This same result is not true for $p < \infty$: for $x = 0, 1, 2$ and $y = 1, 2, 3$, we have $\|x - y\|_p = \sqrt{3}$ whereas $DTW_p(x, y) = \sqrt{2}$. However, the DTW is translation invariant: $DTW_p(x, z) = DTW_p(x + b, z + b)$ and $NDTW_p(x, z) = NDTW_p(x + b, z + b)$ for any scalar $b$ and $0 < p \leq \infty$.

In classical analysis, we have that $n^{1/p - 1/q}\|x\|_q \geq \|x\|_p [47]$ for $1 \leq p < q \leq \infty$. A similar results is true for the DTW and it allows us to conclude that $DTW_p(x, y)$ and $NDTW_p(x, y)$ decrease monotonically as $p$ increases.

Proposition 4 For $1 \leq p < q \leq \infty$, we have that $(2n - 2)^{1/p - 1/q}DTW_q(x, y) \geq
\[ DTW_p(x, y) \] where \( n \) is the length of \( x \) and \( y \). The result also holds for the non-monotonic DTW.

**PROOF.** Assume \( n > 1 \). The argument is the same for the monotonic or non-monotonic DTW. Given \( x, y \) consider the two aligned (and extended) time series \( x', y' \) such that \( DTW_q(x, y) = \|x' - y'\|_q \). Let \( n_{x'} \) be the length of \( x' \) and \( n_{y'} \) be the length of \( y' \). As a consequence of Proposition 3, we have \( n_{x'} = n_{y'} \leq 2n - 2 \). From classical analysis, we have \( n_{1/p} - n_{1/q} \|x' - y'\|_q \geq \|x' - y'\|_p \) or \( 2n_{1/p} - 2n_{1/q} DTW_q(x, y) \geq \|x' - y'\|_p \).

Since \( x', y' \) represent a valid warping path of \( x, y \), then \( \|x' - y'\|_p \geq DTW_p(x, y) \) which concludes the proof.

**B The Triangle Inequality**

The DTW is commonly used as a similarity measure: \( x \) and \( y \) are similar if \( DTW_p(x, y) \) is small. Similarity measures often define equivalence relations: \( A \sim A \) for all \( A \) (reflexivity), \( A \sim B \Rightarrow B \sim A \) (symmetry) and \( A \sim B \land B \sim C \Rightarrow A \sim C \) (transitivity).

The DTW is reflexive and symmetric, but it is not transitive. Indeed, consider the following time series:

\[
X = 0, 0, \ldots, 0, 0, \underbrace{\epsilon, \epsilon, \ldots, \epsilon, \epsilon, 0}_{2m \text{ times}}
\]

\[
Y = 0, 0, \ldots, 0, \underbrace{\epsilon, 0, 0, \ldots, 0, 0}_{m \text{ times}}
\]

\[
Z = 0, 0, \ldots, 0, \underbrace{\epsilon, \epsilon, \ldots, \epsilon, \epsilon, 0}_{2m - 1 \text{ times}}
\]

We have that \( NDTW_p(X, Y) = DTW_p(X, Y) = \|\epsilon\|_1, NDTW_p(Y, Z) = DTW_p(Y, Z) = 0, NDTW_p(X, Z) = DTW_p(X, Z) = \sqrt{(2m - 1)}|\epsilon| \) for \( 1 \leq p < \infty \) and \( w = m - 1 \). Hence, for \( \epsilon \) small and \( n \gg 1/\epsilon \), we have that \( X \sim Y \) and \( Y \sim Z \), but \( X \not\sim Z \). This example proves the following lemma.

**Lemma 3** For \( 1 \leq p < \infty \) and \( w > 0 \), neither \( DTW_p \) nor \( NDTW_p \) satisfies a triangle inequality of the form \( d(x, y) + d(y, z) \geq cd(x, z) \) where \( c \) is independent of the length of the time series and of the locality constraint.

This theoretical result is somewhat at odd with practical experience. Casacuberta et al. found no triangle inequality violation in about 15 million triplets of voice recordings [48]. To determine whether we could expect violations of the triangle inequality in practice, we ran the following experiment. We
used 3 types of 100-sample time series: white-noise times series defined by
\[ x_i = N(0, 1) \] where \( N \) is the normal distribution, random-walk time series
defined by \( x_i = x_{i-1} + N(0, 1) \) and \( x_1 = 0 \), and the Cylinder-Bell-Funnel time
series proposed by Saito [43]. For each type, we generated 100 000 triples of
time series \( x, y, z \) and we computed the histogram of the function
\[ C(x, y, z) = \frac{\text{DTW}_p(x, z)}{\text{DTW}_p(x, y) + \text{DTW}_p(y, z)} \]
for \( p = 1 \) and \( p = 2 \). The DTW is computed without time constraints. Over
the white-noise and Cylinder-Bell-Funnel time series, we failed to find a single
violation of the triangle inequality: a triple \( x, y, z \) for which \( C(x, y, z) > 1 \).
However, for the random-walk time series, we found that 20% and 15% of the
triples violated the triangle inequality for DTW
\[ \text{DTW}_1 \] and DTW
\[ \text{DTW}_2 \].

The DTW satisfies a weak triangle inequality as the next theorem shows.

**Theorem 2** Given any 3 same-length time series \( x, y, z \) and \( 1 \leq p \leq \infty \), we have
\[ \text{DTW}_p(x, y) + \text{DTW}_p(y, z) \geq \frac{\text{DTW}_p(x, z)}{\min(2w + 1, n)^{1/p}} \]
where \( w \) is the locality constraint. The result also holds for the non-monotonic
DTW.

**PROOF.** Let \( \Gamma \) and \( \Gamma' \) be minimal warping paths between \( x \) and \( y \) and be-
tween \( y \) and \( z \). Let \( \Gamma'' = \{(i, j, k) | (i, j) \in \Gamma \text{ and } (j, k) \in \Gamma'\} \). Iterate through
the tuples \((i, j, k) \in \Gamma'' \) and construct the same-length time series \( x'', y'', z'' \)
from \( x_i, y_j, \) and \( z_k \). By the locality constraint any match \((i, j) \in \Gamma \) cor-
responds to at most \( \min(2w + 1, n) \) tuples of the form \((i, j, \cdot) \in \Gamma'' \), and
similarly for any match \((j, k) \in \Gamma' \). Assume \( 1 \leq p < \infty \). We have that
\[ \|x'' - y''\|_p = \sum_{(i, j, k) \in \Gamma''} |x_i - y_j|^p \leq \min(2w + 1, n) \text{DTW}_p(x, y)^p \]
and \[ \|y'' - z''\|_p = \sum_{(i, j, k) \in \Gamma''} |y_j - z_k|^p \leq \min(2w + 1, n) \text{DTW}_p(y, z)^p. \]
By the triangle inequality in \( l_p \), we have
\[ \min(2w + 1, n)^{1/p} (\text{DTW}_p(x, y) + \text{DTW}_p(y, z)) \geq \|x'' - y''\|_p + \|y'' - z''\|_p \]
\[ \geq \|x'' - z''\|_p \geq \text{DTW}_p(x, z). \]

For \( p = \infty \), \[ \max_{(i, j, k) \in \Gamma''} \|x_i - y_j\| = \text{DTW}_\infty(x, y)^p \] and \( \max_{(i, j, k) \in \Gamma''} |y_j - z_k|^p = \text{DTW}_\infty(y, z)^p \), thus proving the result by the triangle inequality over \( l_\infty \). The
proof is the same for the non-monotonic DTW.

The constant \( \min(2w + 1, n)^{1/p} \) is tight. Consider the example with time series
\( X, Y, Z \) presented before Lemma 3. We have \( \text{DTW}_p(X, Y) + \text{DTW}_p(Y, Z) = |\epsilon| \)
and $\DTW_p(X, Z) = \sqrt[2w + 1]{|\epsilon|}$. Therefore, we have

$$\DTW_p(X, Y) + \DTW_p(Y, Z) = \frac{\DTW_p(X, Z)}{\min(2w + 1, n)^{1/p}}.$$

A consequence of this theorem is that $\DTW_\infty$ satisfies the traditional triangle inequality.

**Corollary 3** The triangle inequality $d(x, y) + d(y, z) \geq d(x, z)$ holds for $\DTW_\infty$ and $\NDTW_\infty$.

Hence the $\DTW_\infty$ is a pseudometric: it is a metric over equivalence classes defined by $x \sim y$ if and only if $\DTW_\infty(x, y) = 0$. When no locality constraint is enforced ($w \geq n$), $\DTW_\infty$ is equivalent to the discrete Fréchet distance [49].

C Which is the Best Distance Measure?

The DTW can be seen as the minimization of the $l_p$ distance under warping. Which $p$ should we choose? Legrand et al. reported best results for chromosome classification using $\DTW_1$ [13] as opposed to using $\DTW_2$. However, they did not quantify the benefits of $\DTW_1$. Morse and Patel reported similar results with both $\DTW_1$ and $\DTW_2$ [50].

While they do not consider the DTW, Aggarwal et al. [51] argue that out of the usual $l_p$ norms, only the $l_1$ norm, and to a lesser extend the $l_2$ norm, express a qualitatively meaningful distance when there are numerous dimensions. They even report on classification-accuracy experiments where fractional $l_p$ distances such as $l_{0.1}$ and $l_{0.5}$ fare better. François et al. [52] made the theoretical result more precise showing that under uniformity assumptions, lesser values of $p$ are always better.

To compare $\DTW_1$, $\DTW_2$, $\DTW_4$ and $\DTW_\infty$, we considered four different synthetic time-series data sets: Cylinder-Bell-Funnel [43], Control Charts [44], Waveform [53], and Wave+Noise [54]. The time series in each data sets have lengths 128, 60, 21, and 40. The Control Charts data set has 6 classes of time series whereas the other 3 data sets have 3 classes each. For each data set, we generated various databases having a different number of instances per class: between 1 and 9 inclusively for Cylinder-Bell-Funnel and Control Charts, and between 1 and 99 for Waveform and Wave+Noise. For a given data set and a given number of instances, 50 different databases were generated. For each database, we generated 500 new instances chosen from a random class and we found a nearest neighbor in the database using $\DTW_p$ for $p = 1, 2, 4, \infty$ and
Fig. C.1. Classification accuracy versus the number of instances of each class in four data sets using a time constraint of $w = n/10$. When the instance is of the same class as the nearest neighbor, we considered that the classification was a success.

The average classification accuracies for the 4 data sets, and for various number of instances per class is given in Fig. C.1. The average is taken over 25 000 classification tests (50 × 500), over 50 different databases.

Only when there are one or two instances of each class is DTW$_\infty$ competitive. Otherwise, the accuracy of the DTW$_\infty$-based classification does not improve as we add more instances of each class. For the Waveform data set, DTW$_1$ and DTW$_2$ have comparable accuracies. For the other 3 data sets, DTW$_1$ has a better nearest-neighbor classification accuracy than DTW$_2$. Classification with DTW$_4$ has almost always a lower accuracy than either DTW$_1$ or DTW$_2$.

Based on these results, DTW$_1$ is a good choice to classify time series whereas DTW$_2$ is a close second.