



22nd ACM SIGKDD Conference on Knowledge Discovery and Data Mining August 13 - 17, 2016 | San Francisco, California

Extracting Optimal Performance from Dynamic Time Warping

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Please cite as: Abdullah Mueen, Eamonn J. Keogh: Extracting Optimal Performance from Dynamic Time Warping. KDD 2016: 2129-2130

Acknowledgements

 The following people helped with advice or images: Diego Silva, Hoang Anh Dau, Tony Bagnall, Mohammad Shokoohi-Yekta, Bing Hu, Chotirat (Ann) Ratanamahatana, François Petitjean (If we forgot anyone, apologies)

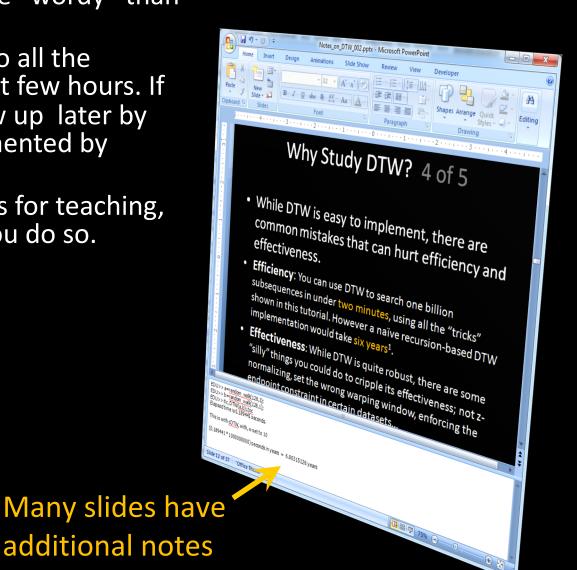
 We also acknowledge the following sponsors and funding agencies: MERL Labs, Samsung, Siemens, Google, MSR/IARPA, NSF IIS-1161997 II and SHF-1527127



 However any errors or opinions are solely due to A.M and E.K

Disclaimer

- Some of the slides are more "wordy" than we would like.
- Our idea is to expose you to all the important issues in the next few hours. If you need to, you can follow up later by re-reading the slides (augmented by notes/references)
- Feel free to use these slides for teaching, but please let us know if you do so.



Approximate Outline

 The First Act: How to do DTW correctly Keogh

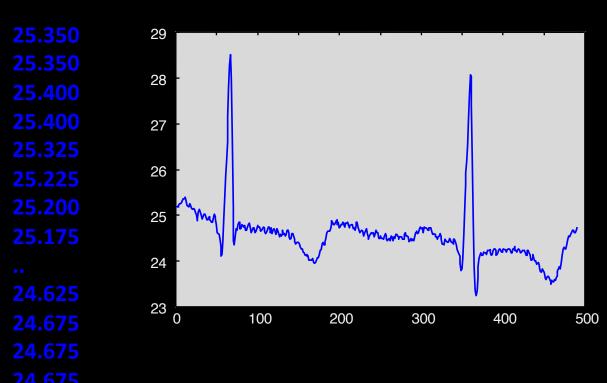
• The Second Act: How to do DTW *fast*Mueen

What are Time Series? 1 of 2

A time series is a collection of observations made sequentially in time.

More than most types of data, time series lend themselves to *visual* inspection and intuitions...

For example, looking at the numbers in this blue vector tells us nothing. But after *plotting* the data, we can recognize a heartbeat, and possibly even diagnose this person's disease. This tutorial will leverage the visual intuitiveness time series.

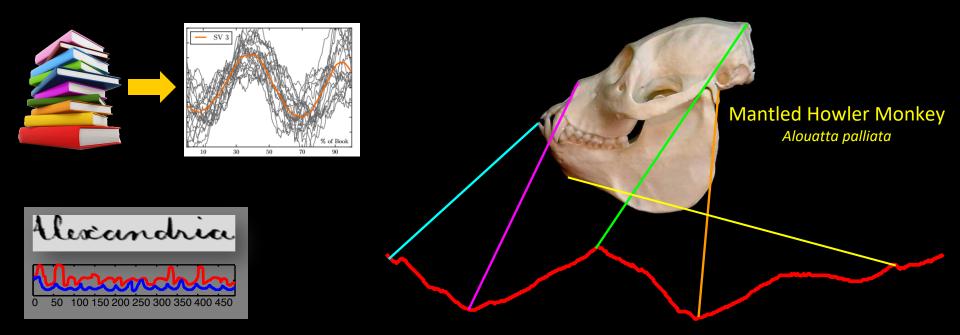


What are Time Series? 2 of 2

As an aside... (not the main point for today)

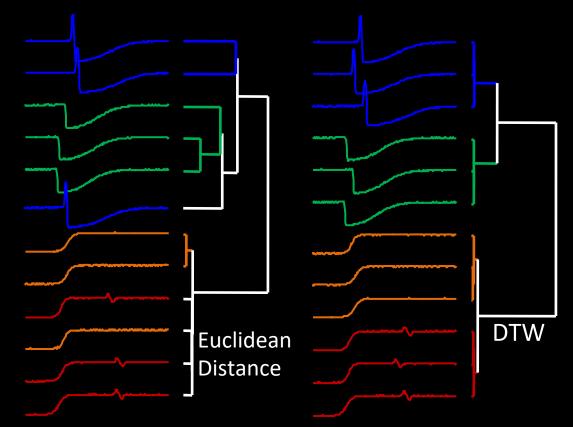
Many types of data that are not *true* time series can be fruitfully transformed into time series, including DNA, speech, textures, core samples, ASCII text, historical handwriting, novels and even *shapes*.

This fact greatly expands the purview of DTW



What is Dynamic Time Warping?

- DTW is an algorithm for measuring similarity between two time series which may vary (i.e. *warp*) in timing.
- This invariance to warping is critical in many domains, for many tasks.
- Without warping invariance, we are often condemned to very poor results.



Why Study DTW? 1 of 5

- Why should you spend several hours studying DTW?
- On the face of it, this *seems* strange.
- We probably would not spend hours on just the Hamming distance, or the just the Jaccard similarity etc.

Why Study DTW? 2 of 5

- It is almost impossible to overstate the ubiquity of DTW in data analytics
- It is used in: robotics, biometrics, medicine, metrology, bioinformatics, video games, gesture recognition, image processing, seismology, music processing, entomology, anthropology, computational photography, bioacoustics, finance,...

Why Study DTW? 3 of 5

- While the is no free lunch, multiple rigorous independent studies¹ show that for the core problem of time series classification, Nearest Neighbor DTW is very hard to beat.
- Moreover, where NN-DTW can be beaten, it typically by a very small margin, at the cost of huge effort in coding/complexity of implementation, and a large time and space overhead.

¹This paper conducts 35 million experiments, on 85 datasets, with dozens of rival methods http://arxiv.org/abs/1602.01711 The Great Time Series Classification Bake Off. Bagnall et al.

Why Study DTW? 4 of 5

- While DTW is easy to implement, there are common mistakes that can hurt efficiency and effectiveness.
- **Efficiency**: You can use DTW to search one billion subsequences in under two minutes, using all the "tricks" shown in this tutorial. However a naïve off-the-shelf recursion-based DTW implementation would take six years¹.
- **Effectiveness**: While DTW is quite robust, there are some "silly" things you could do to cripple its effectiveness; not z-normalizing, set the wrong warping window, enforcing the endpoint constraint in certain datasets...

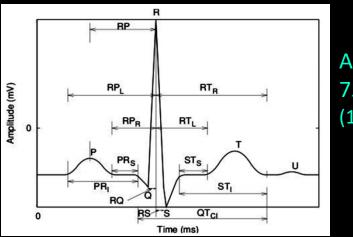
Why Study DTW? 5 of 5

- Finally, many of the ideas we will discuss today to make DTW effective and efficient, can be applied to other domains. (constraining distance measures that are "too" invariant, lower bounding search, just-in-time normalization, early abandoning, cascading multiple lower bounds...)
- So, even if you don't care about DTW per se, we hope you will find some ideas you can use.

An Unstated Assumption

For all time series, faces, gait, fish and heartbeats, we could design and extract features, and just represent the objects as feature vectors. However, in the dozens of cases where we compared this type of approach to just using DTW on the raw data, DTW almost always wins!

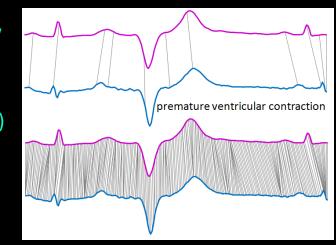
So, at the very least, try the simplest ideas first, and DTW is very simple.



Bazett's formula

Accuracy 75 to 95% (10 classes)

1NN DTW Accuracy 98% plus (10 classes)



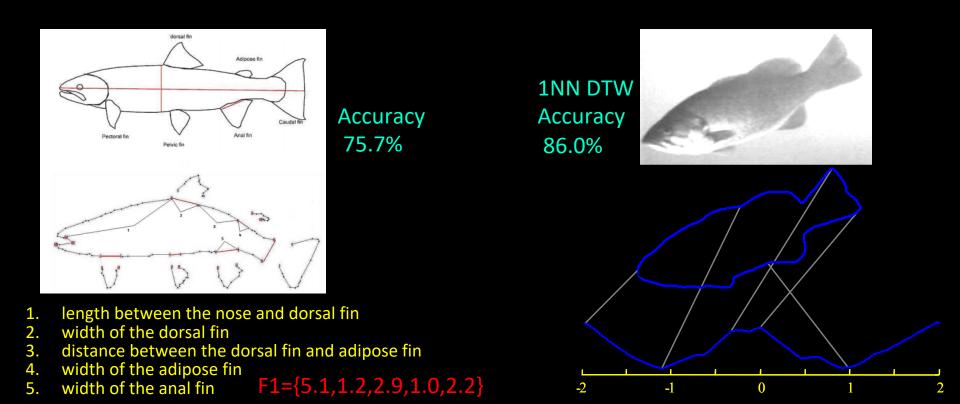
PR Interval, PR Segment, Corrected-QT Interval, ST Segment , ST Interval , RR Interval , RQ Amplitude, R_{peak} to T_{onset} Segment RS Amplitude , Angle Q, Angle R, Angle S,... F1={7.3,4.2,5.2,1.2,6.7, ...}

Parameter-free or parameter-lite, robust to noise etc.

An Unstated Assumption (alterative)

For all time series, heartbeats, gait, faces, and even fish!, we could design and extract features, and just represent the objects as feature vectors. However, in the dozen of cases where we compared this type of approach to just using DTW on the raw data, DTW almost always wins!

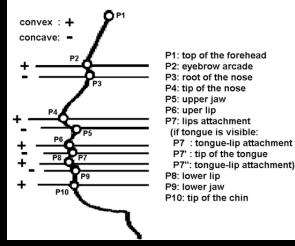
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An Unstated Assumption (alterative)

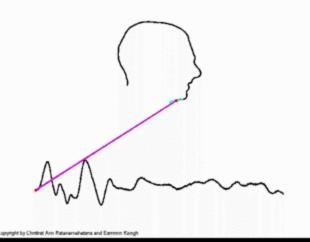
For all time series, heartbeats, gait, fish and faces, we could design and extract features, and just represent the objects as feature vectors. However, in the dozen of cases where we compared this type of approach to just using DTW on the raw data, DTW almost always wins!

So, at the very least, try the simplest ideas first, and DTW is very simple.



Accuracy 70 to 80% (10 classes) P7 : tongue-lip attachment

1NN DTW Accuracy 90% plus (10 classes)



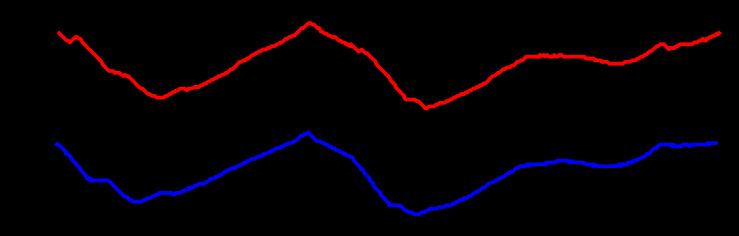
Parameter-free or parameter-lite, robust to changes of expression...

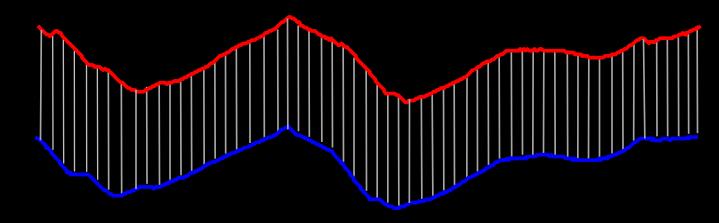
How many fiducials? Pantic suggests 10, Campos suggests 8, Dariush suggests 9, Liposcak suggests 12...

F1={7.4,1.3,2.1,1.2,4.6, 5.6, 43.3}

A Visual Intuition of Distance Measures

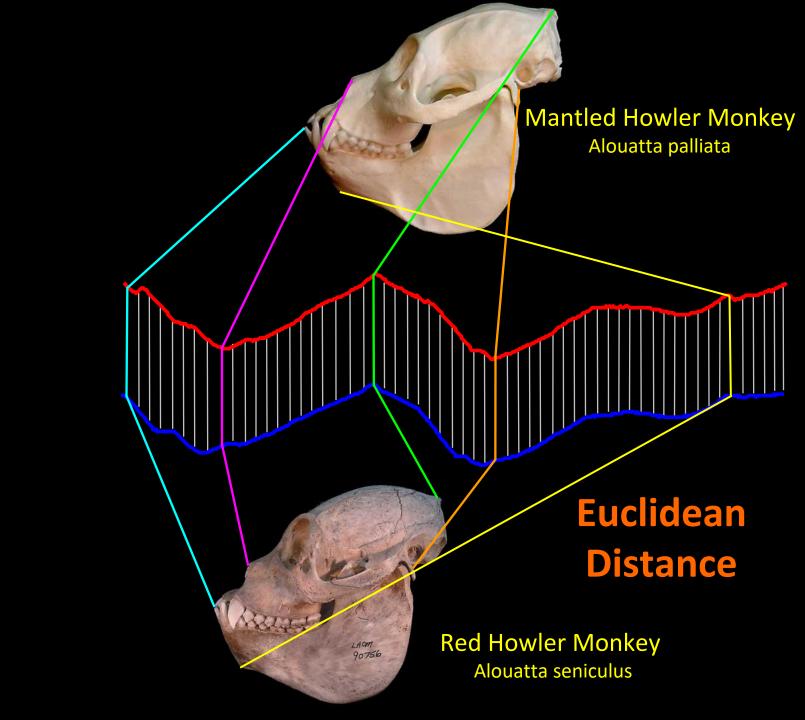
We have two time series, what is the distance between them? Equivalently, how similar are they?

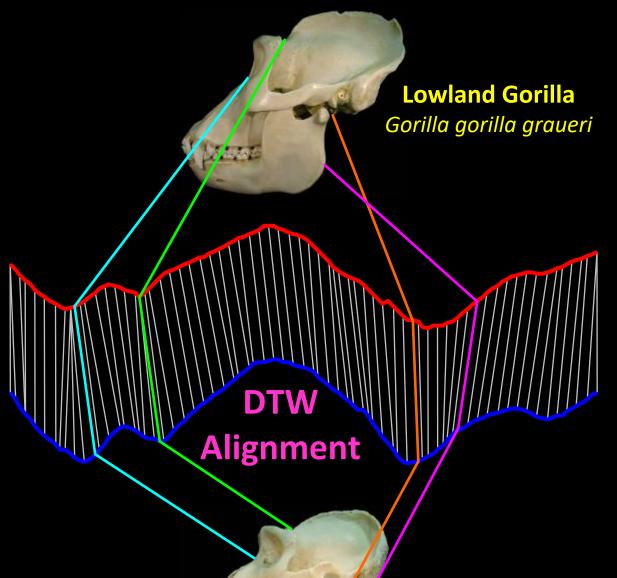




Euclidean Distance

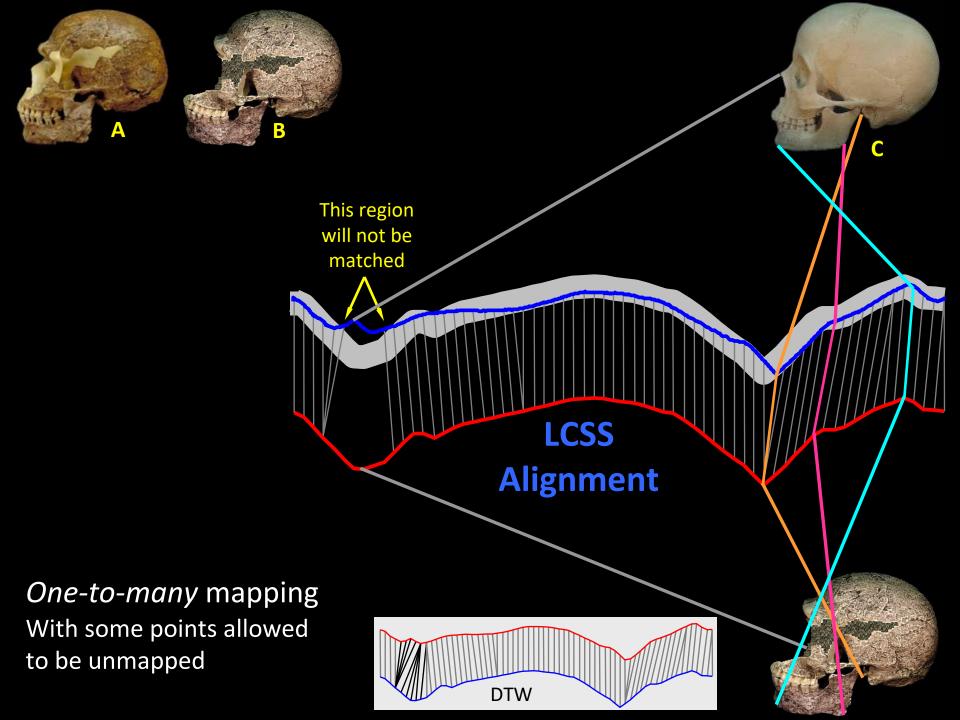
One-to-one mapping





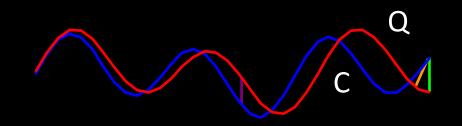
One-to-many mapping

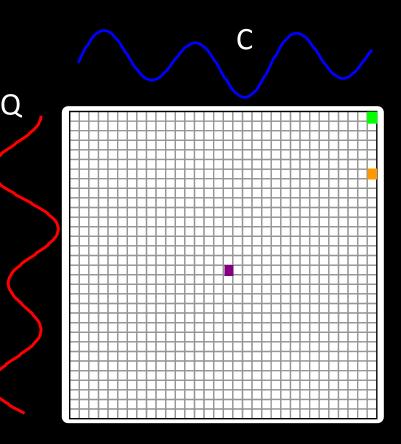




How is DTW Calculated? I

We create a matrix the size of |Q| by |C|, then fill it in with the distance between every possible pair of points in our two time series.



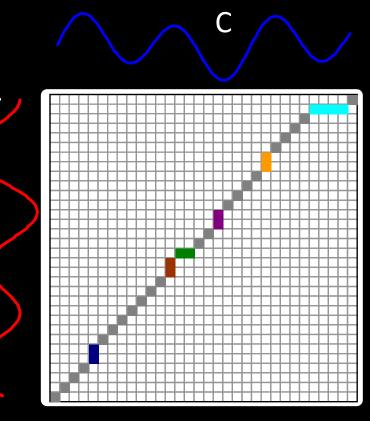


How is DTW Calculated? II

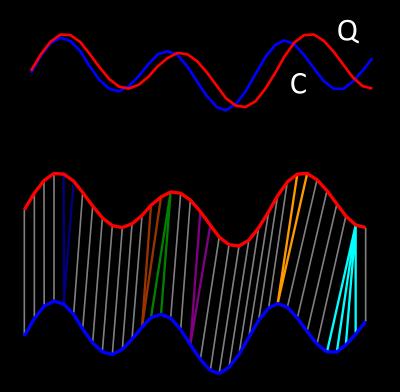
Every possible warping between two time series, is a path through the matrix. We want the *best* one...

Q

$$DTW(Q,C) = \min\left\{\sqrt{\sum_{k=1}^{K} w_k} \middle| K\right\}$$



Warping path w



This recursive function gives us the minimum cost path

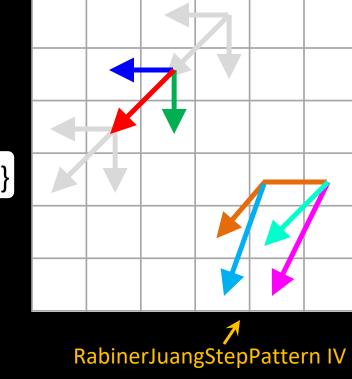
$$\gamma(\mathbf{i},\mathbf{j}) = d(q_{\mathbf{i}},c_{\mathbf{j}}) + \min\{\gamma(\mathbf{i}-1,\mathbf{j}-1),\gamma(\mathbf{i}-1,\mathbf{j}),\gamma(\mathbf{i},\mathbf{j}-1)\}$$

We can visualize the recursive function as a "step pattern" of allowable moves, or search operators

 $\gamma(i,j) = d(q_i,c_j) + \min\{\gamma(i-1,j-1), \gamma(i-1,j), \gamma(i,j-1)\}$

This suggests two generalizations.

- We could weight the diagonal step, to "discourage" the warping path wandering too far from the diagonal.
- We could create other steps patterns, including asymmetric step patterns.



Both ideas were extensively studied when DTW was the dominant speech processing algorithm, but have not been investigated extensively in the data mining context. Empirically, they seem to make little difference. We only consider the classic symmetric1 step pattern in our work.

How is DTW Calculated? Disclaimer!

In practice we **don't** use *recursion* to calculate DTW. Instead we use an equivalent *iterative* method (which we will explain later).

The iterative method is both absolutely faster, and it is allows many speed-up optimizations (early abandoning etc).

The time difference is several orders of magnitude.

However, there is no logical difference between the two methods for the first half of this tutorial.

This recursive function gives us the minimum cost path

$$\gamma(i,j) = d(q_i,c_j) + \min\{\gamma(i-1,j-1), \gamma(i-1,j), \gamma(i,j-1)\}$$

Logically correct, but too slow and memory intensive

DTW is a Distance *Measure*, not a *Metric* 1 of 2

Requirements to be a metric

Yes for DTWD(A,B) = D(B,A)SymmetryD(A,A) = 0Constancy of Self-SimilarityD(A,B) = 0 IIf A=BPositivity (Separation)No for DTW $D(A,B) \le D(A,C) + D(B,C)$ Triangular Inequality

Normally we prefer metrics over measures for two reasons:

• Non-Metrics can sometimes give pathological solutions when clustering or classifying data etc.

 Almost all speed-up "tricks" for high dimensional data exploit the Triangular Inequality.

DTW is a Distance *Measure*, not a *Metric* 2 of 2

• Non-Metrics can sometimes give pathological solutions when clustering or classifying data etc.

DTW is *almost* a metric! That is to say if you randomly sample a million triples A, B and C, you will probably find $D(A,B) \le D(A,C) + D(B,C)$ is obeyed for 999,999 of them.

*Moreover, in the limit, as *w* approaches zero, DTW *is* a metric. As we will see, we almost always use a very small value of *w*.

• Almost all speed-up "tricks" for high dimensional data exploit the Triangular Inequality.

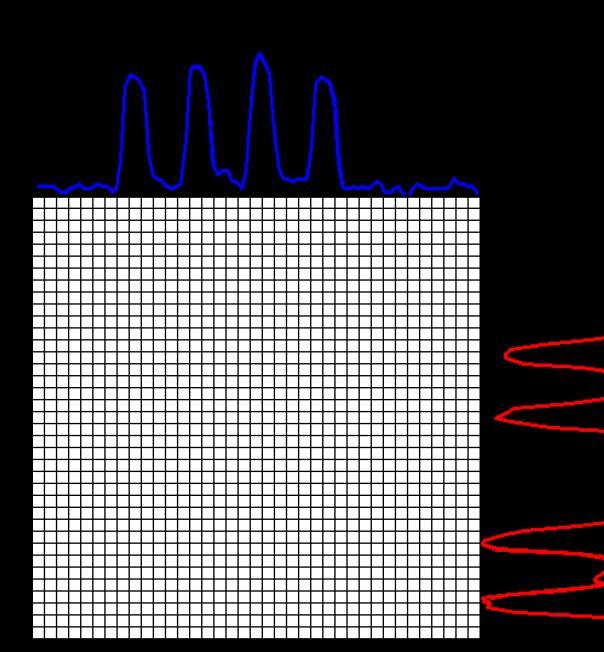
This used to be a big issue, but after a decade of research, the community has found alterative techniques that allow us to speed up DTW (Second half of the tutorial).

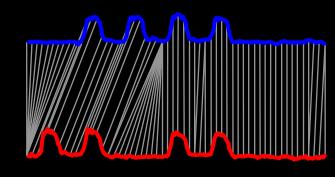
*We will explain what "w" is in a <u>few slides</u>.

DTW: Time and Space complexity

- The "off-the-shelf" DTW has
- a time complexity of $O(n^2)$ (with a large constant factor)
- a space complexity of $O(n^2)$ This is the most cited reason for not using DTW.
- However, as we will show in the second half of this tutorial. DTW can have
- a space complexity of O(n)
- an amortized time complexity of O(n) (with a very small constant factor)

Let us visualize the cumulative matrix on a real world problem I

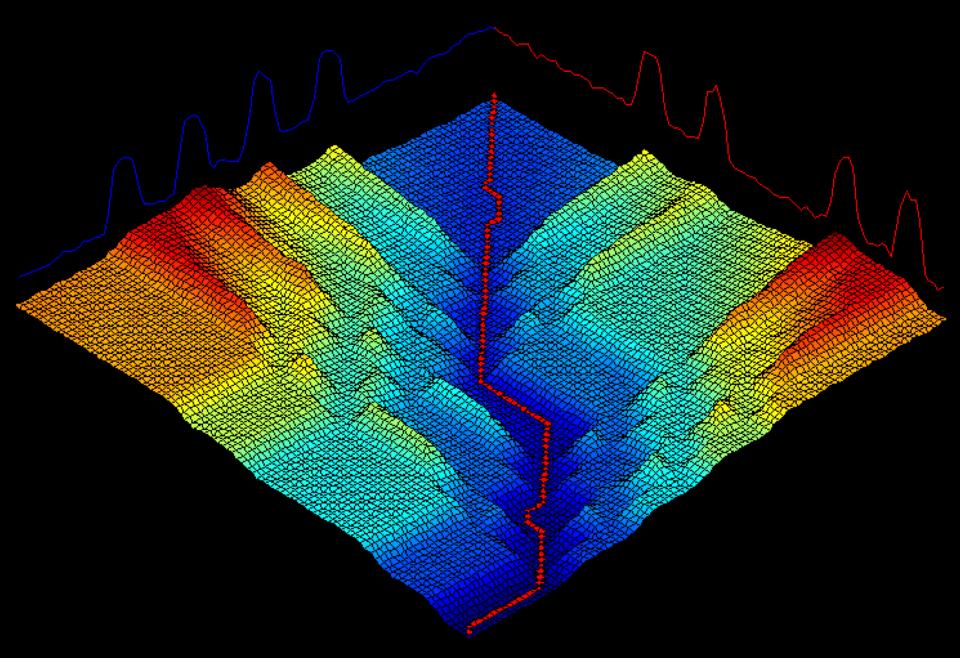




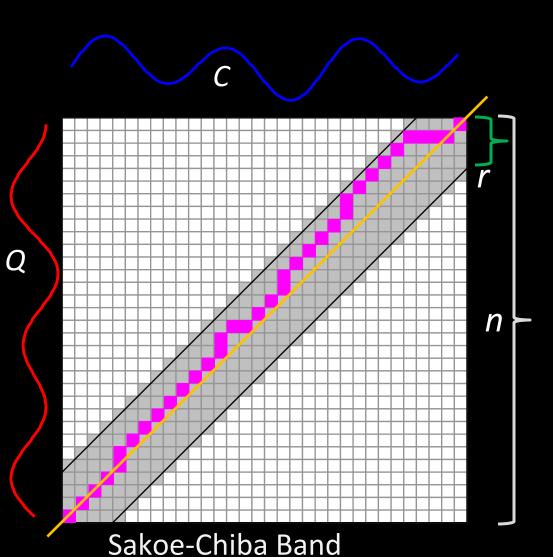
This example shows two one-week periods from an electrical power demand time series.

Note that although they both describe 4-day work weeks, the blue sequence had Monday as a holiday, and the red sequence had Wednesday as a holiday.

Let us visualize the cumulative matrix on a real world problem II



Understanding w, the Warping Constraint



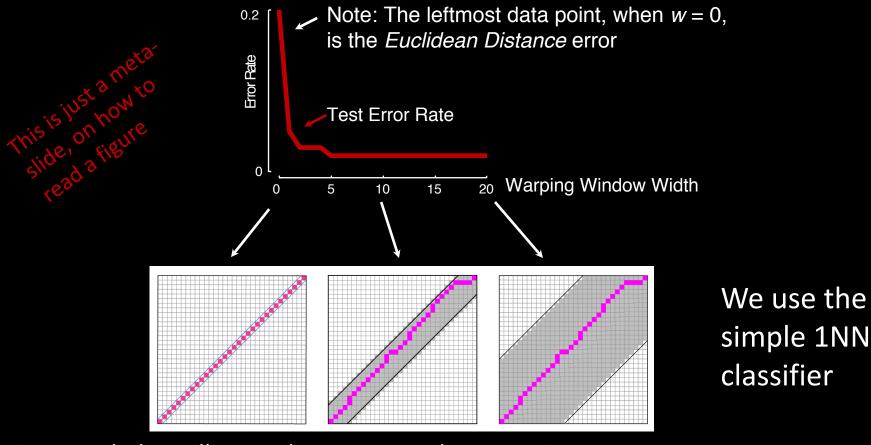
The value of w is the maximum amount the warping path is allow to deviate from the diagonal. It is normally expressed as the ratio W = r/n (or as a percentage)

We need to understand *w* because:

- The most useful speedup tricks all exploit *w*.
- The value chosen for *w* can greatly affect accuracy.

Preamble: Reading the plots for.. The value of *w* vs. some measure of quality

Testing every value of w, from w = 0 to w = 20



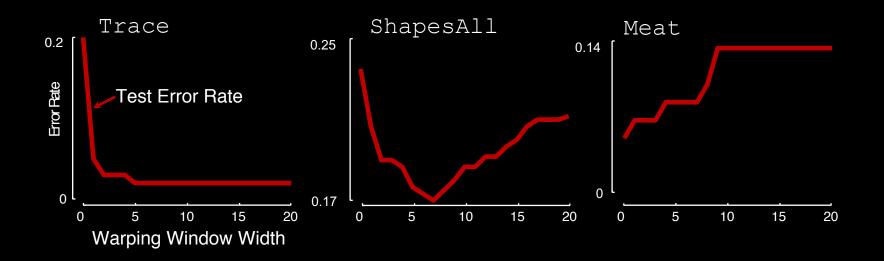
Time needed: Milliseconds,....

Seconds,....

Minutes,... (at least, if naively implemented)

How important is the value of w?

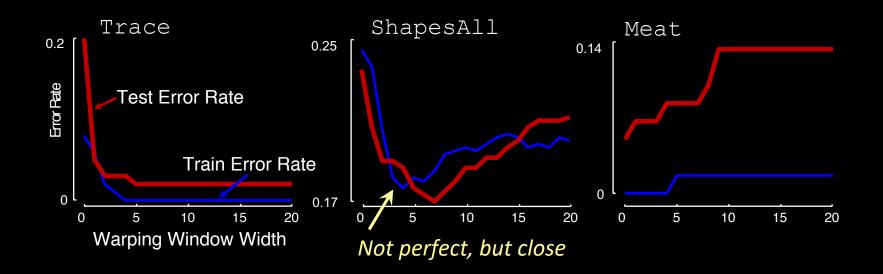
To find out, we measured the testing accuracy on some UCR datasets We tested every value of w, from w = 0 to w = 20



There is high variability: Any warping *hurts* for Meat (such datasets are rare), any amount of warping above 5 is optimal for Trace, and ShapesAll really needs 7, not more, not less. How can we set the value of *w*?

How can we set the value of w?

We can set the value of *w* using leave-one-out cross-validation on the testing data. So long as we have enough labeled data, this generally works very well, as shown below:



What do you do if you don't have enough labeled data? (open problem) One Idea: Find a dataset that is similar, that *does* have labeled data, and hope the best setting generalizes from that dataset.

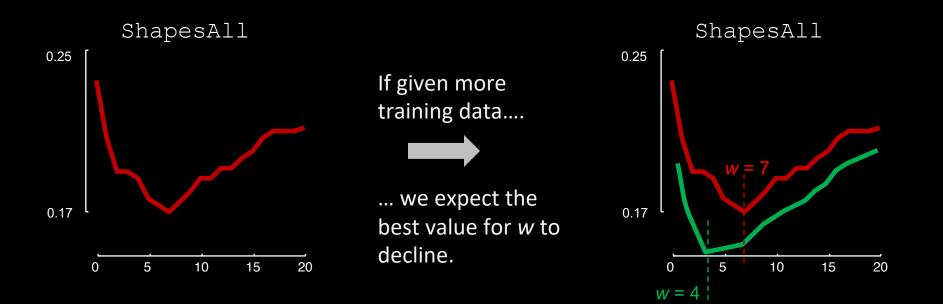
The value of w vs. data size

For classification and query-by-content, the best setting of *w* also depends on the *size* of the training dataset.

If we are given more training data, we should expect:

- The error rate to decrease (as with all ML problems and all data types)
- The best value for w to get smaller (it is possible to construct synthetic counterexamples)

This implies that with enough training data, you would not need DTW!



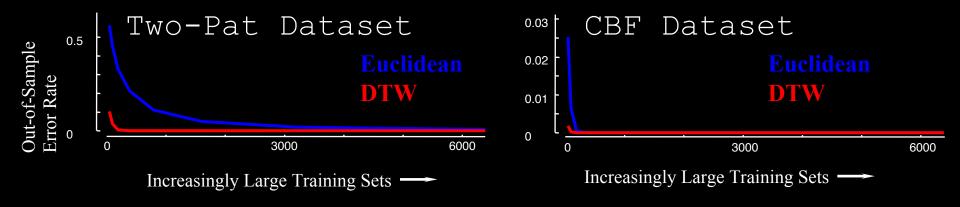
..this implies that with enough training data, you would not need DTW!

Empirically, these seems to be universally true. 1NN-DTW classification is generally much more accurate than 1NN-ED classification for small datasets. However, as you add more training data, the gap begins to close, and eventually converges.

To our knowledge, there is no research on quantifying how fast they converge, if they must converge, the relative benefit of a new training object for each approach etc.

As a practical matter, this observation probably does not matter much.

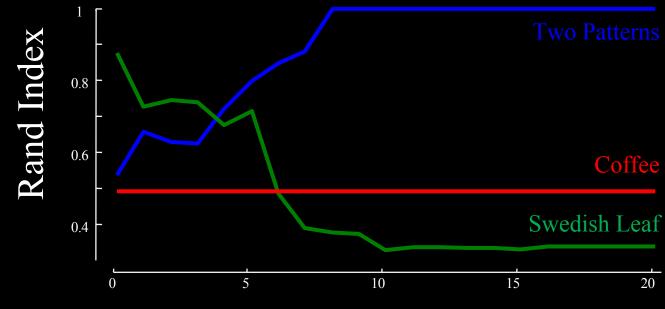
- We rarely have the luxury lots of training data
- If we did, it would probably still be faster to do 1NN-DTW with less data, than 1NN-ED with lots of data.



Revisited: How important is the value of w? 1 of 5

While the community has just begun to understand that the setting of *w* is important for *classification*, it is not well appreciated that it is just as important for *clustering*.

Below we show the rand-index vs *w* for three datasets, clustered using TADPole. As we can see, the value of *w* is critical.

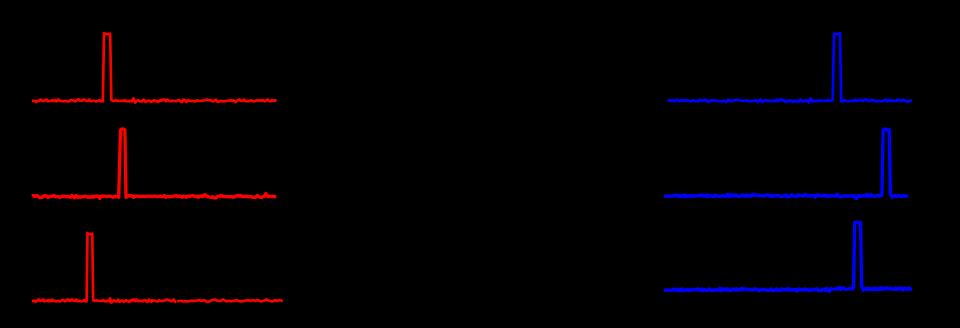


Warping Window Width (as % of time series length)

Revisited: How important is the value of w? 2 of 5

Why is the value of *w* is so critical? The Goldilocks Principle

Lets *make* a dataset of time series of length 100. The dataset is mostly a flat line with a little noise. The red class has a single "spike" somewhere between 1 and 40. The blue class has a single "spike" somewhere between 60 and 100.

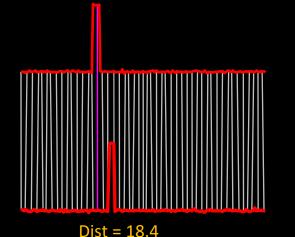


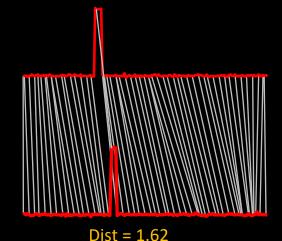
Revisited: How important is the value of w? 3 of 5

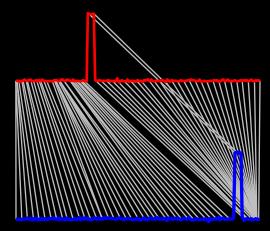
Why is the value of *w* is so critical? The Goldilocks Principle

Lets *make* a dataset of time series of length 100. The dataset is mostly a flat line with a little noise. The red class has a single "spike" somewhere between 1 and 40. The blue class has a single "spike" somewhere between 60 and 100.

With *no* warping allowed, we map the top of the spike on the source to a low spot on the target. With *a little* warping allowed, we map the spike on the source to spike on the target. Success! With *unlimited* warping allowed, we can map the top of the spike on the source to a very far away spike, which what defines the opposite class!







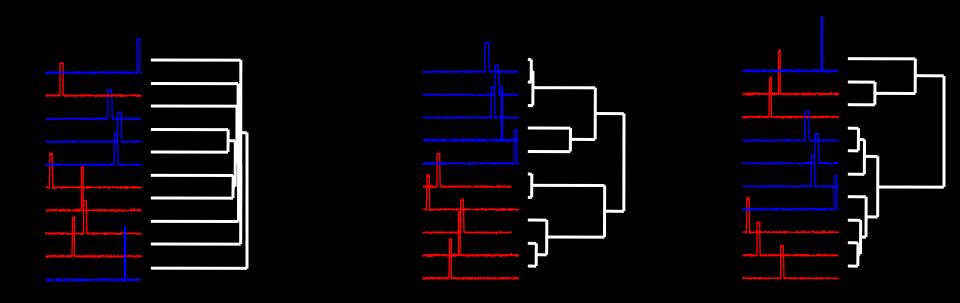


Revisited: How important is the value of w? 4 of 5

Why is the value of *w* is so critical? The Goldilocks Principle

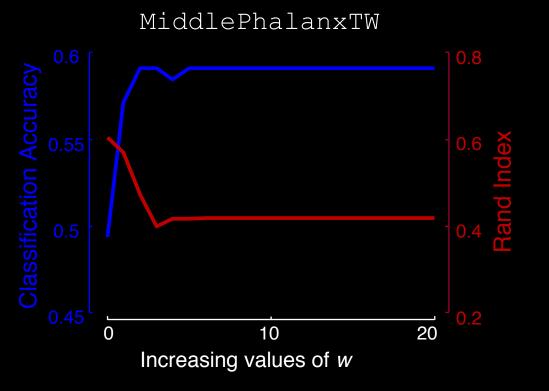
Lets *make* a dataset of time series of length 100. The dataset is mostly a flat line with a little noise. The red class has a single "spike" somewhere between 1 and 40. The blue class has a single "spike" somewhere between 60 and 100.

- With no warping allowed, we get random results
- With a little warping allowed (say 10%), a red can "warp" to a red, and vice versa
- With 100% warping allowed, a blue could warp to a red, and vice versa.



Revisited: How important is the value of w? 5 of 5

Important note: The best value of *w* for **classification** may not be the best value for **clustering**.



In retrospect it is not surprising that these values are at best weakly related. For 1NN classification only the distance between the unlabeled exemplar and it's *single* nearest neighbor matters.

However, for clustering, the mutual distance among small *groups* of objects matter.

The Rand-Index and the classification accuracy vs. the warping window width, for the MiddlePhalanxTW dataset.

Time series of different lengths 1 of 2

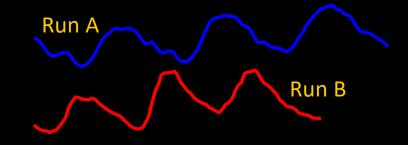
What if you have two time series that are different lengths? For example, here Run B is only 81% the length of Run A.

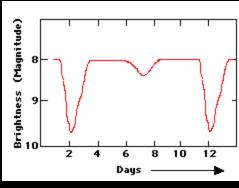
This situation occurs quite a lot:

- Heartbeats recorded at 60bpm vs. 50bpm
- Star light curves come in discrete classes, but each class can have variable periods.
- An utterance of '*Mississippi*' may take 0.6 to 0.9 seconds

– Etc.

This *global* difference in scaling is typically independent of the *local* scaling that DTW is designed to handle.





Star light curve

Time series of different lengths 2 of 2

What if you have two time series that are different lengths? For example, here B is only 81% the length of A.

There are at least two things you can do:

1) Compare them in their native lengths.

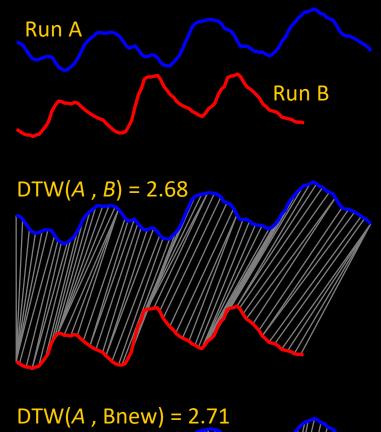
2) Re-interpolate them to have the same length.

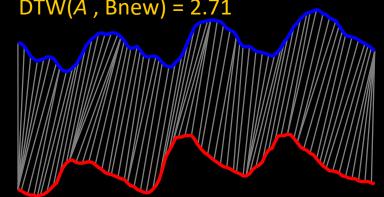
An inelegant, but quick way to do this in Matlab is:

Bnew= B(1:0.81:end);

Empirically makes little or no difference for classification, clustering etc.

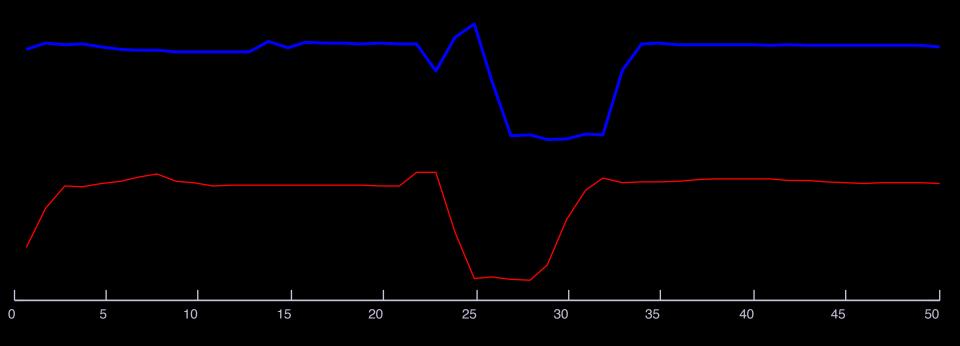
However, the equal length case is much easier to handle, so we assume it from now on.





The Importance of Endpoints: 1 of 3

Consider the two time series below. They are similar, but out of phase, *exactly* the case that DTW is designed for. <u>Let us compare them using DTW....</u>



Thanks to Diego Silva for help with this example

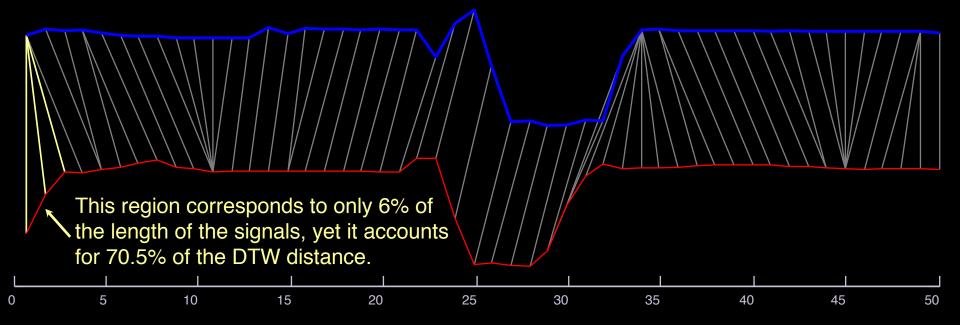
The Importance of Endpoints: 2 of 3

DTW *can* be invariant to all the warping, but it cannot handle the difference at the very beginning of these two time series. Recall the boundary constraint:

Boundary Condition: $w_1 = (1,1)$ and $w_K = (m,n)$, this requires the warping path to start and finish in

diagonally opposite corner cells of the matrix.

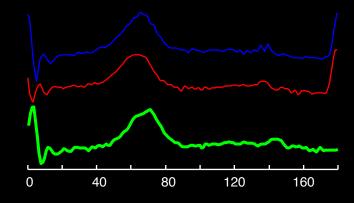
This constraint means that DTW must match the pairs of *beginning* (and *end*) points, even though they may be a poor match, as here.



The Importance of Endpoints: 3 of 3

Possible Fixes (Open problem)

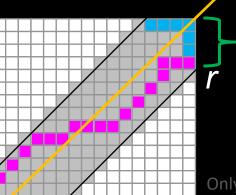
1) Use a better subsequence extraction algorithm. For example, the heartbeats to the right were very badly extracted, and have a large variability in the endpoints.



2) Recall the warping path is:

 $W = w_1, w_2, w_3, \dots w_{K-2}, w_{K-1}, \dots, w_K$

If you fear that the error is concentrated at the ends, you can multiple the first and last r elements by a weight \hat{W} , with $0 \le \hat{W} \le 1$

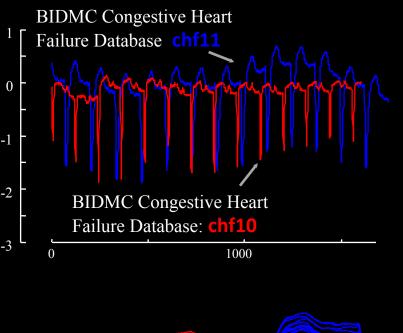


- 3) Open-Ended Warping: Redefine the endpoint constraint. Change... Boundary conditions: $w_1 = (1,1)$ and $w_{\kappa} = (m,n)$, this requires the warping path to start and finish in diagonally opposite corner cells of the matrix.
- ...to

Boundary conditions: $w_1 = (1,B)$ or (B,1) and $w_{\kappa} = (m-C,n)$ or (m,n-C), with $0 \le B \le r$, and $0 \le C \le r$ this requires the warping path to start and finish in a cyan cell.

Only top right section of the warping matrix shown for brevity

The Importance of Z-Normalization 1 of 3



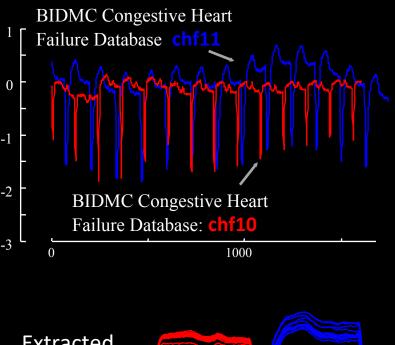
Extracted beats chf10 chf11

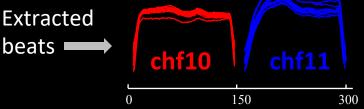
Essentially all datasets must have *every* subsequence z-normalized. There are a handful of occasions where it does not make sense to z-normalize, but in those cases, DTW probably does not make sense either.

In this example, we begin by extracting heartbeats from two unrelated people.

Even without normalization, it happens that both sets have almost the same mean and standard deviation. Given that, do we need to bother to normalize them? (next slide)

The Importance of Z-Normalization 2 of 3



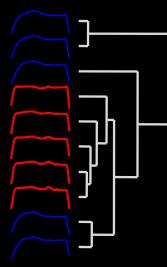


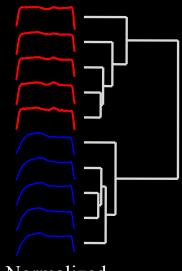
In this example, we extracted heartbeats from two different time series, and clustered them with and without normalization.

Surprisingly z-normalizing can be a computational bottleneck, but later we will show you how to fix that.

Without normalization, the results are *very* poor, some blue heartbeats are closer to red heartbeats than there are to another blue beat .

With normalization, the results are perfect.





Un-normalized

Normalized

The Importance of Z-Normalization 3 of 3

Preempting a common misunderstanding

It is *not* sufficient to normalize the entire time series. You must normalize <u>each</u> subsequence

While there are a handful of normalization techniques , in most cases z-normalizing seems best: T = (T-mean(T))/std(T)

Consider for example the famous Gun/Point dataset. Do we need to normalize it?

- Not as it stands... ...but suppose
- The camera pans down? (the mean changes)
- The camera zooms out? (the STD changes)
- The actor wears high heel shoes? (the mean changes)
- We find a shorter actor? (the mean and the STD change)



Lots of papers claim to be able to beat 1NN-DTW, is that true? Hmm..., no and yes.

• No: More than 90% of such claims are false to cherrypicking, training and testing on the same data, the Texas Sharpshooter fallacy (see next slide), etc

• Yes: There are a *handful* of such methods, but...

-They sometimes win, but typically by very slim margins (say 1 to 3% better).

-They come at a huge cost of coding effort, time complexity.

– They just beat the most basic 1NN-DTW, with the simple CV trick to learn the warping window. It is less clear they could beat KNN-DTW, when a little more effort was spent to find a good warping window.

–We strongly recommend the bake-offs/discussion by Dr. Tony Bagnall.

At a minimum, it is clear that 1NN-DTW will get you within 98% of the best accuracy possible, in the first five minutes.

The Texas Sharpshooter Fallacy

- A paper in SIGMOD 2016 claims "Our STS3 approach is more accurate than DTW in our suitable scenarios".
- They then note "DTW outperforms STS3 in 79.5% cases." !?! (our emphasis)
- They then do a *post-hoc* explanation of why they *think* they won on 20.5% of the cases that "suit them".
- The problem is the *post-hoc* analysis, this is a form of the Texas Sharpshooter Fallacy. Below is a visual representation.

This is what they show you, and you are impressed...



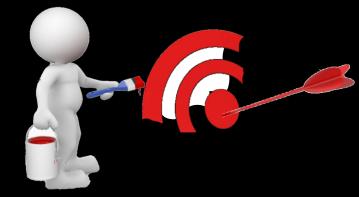
The Texas Sharpshooter Fallacy

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This is what they show you, and you are impressed...



...until you realize that they shot the arrow first, and then painted the target around it!



A good visual trick to compare algorithms of the 80 or so labeled time series in the public domain is the Texas Sharpshooter plot.

For each dataset

• First you compute the baseline accuracy of the approach you hope to beat.

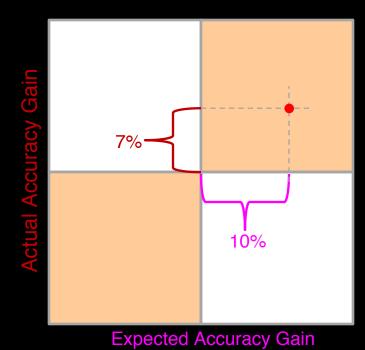
• Then you compute the **expected improvement** we would get using your proposed approach (at this stage, learning any parameters and settings) using *only* the training data. Note that the expected improvement could be negative.

• Then compute the actual improvement obtained (using these now hardcoded parameters and settings) by testing on the test dataset.

You can plot the point {expected improvement , actual improvement } in a 2D grid, as below.

In this example, we predicted the expected improvement would be 10%, and the actual improvement obtained was 7%, pretty close!

We need to do these for all 80 or so datasets. What are the possible outcomes?



Can you beat 1NN-DTW? 3 of 3

With a Texas Sharpshooter plot, each dataset falls into one of four possibilities.

- We expected an improvement and we got it! This is clearly the best case.
- We expected to do worse, and we did. This is *still* a good case, we know not to use our proposed algorithm for these datasets
- We expected to do worse, but we did better. This is the wasted opportunity case.
- We expected to do better, but actually did worse. This is the worst case.

Now that we know how to read the plots, we will use it to see if DTW is better than Euclidean Distance,

Expected Improvement: We will search over different warping window constraints, from 0% to 100%, in 1% increments, looking for the warping window size that gives the highest 1NN training accuracy (if there are ties, we choose the smaller warping window size).

Actual Improvement: Using the warping window size we learned in the last phase, we test the holdout test data on the training set with 1NN.

Texas Sharpshooter Plot

We expected to do worse, but we did better	We expected an improvement and we got it!
We expected to do worse, and we did	We expected to do better, but actually did worse

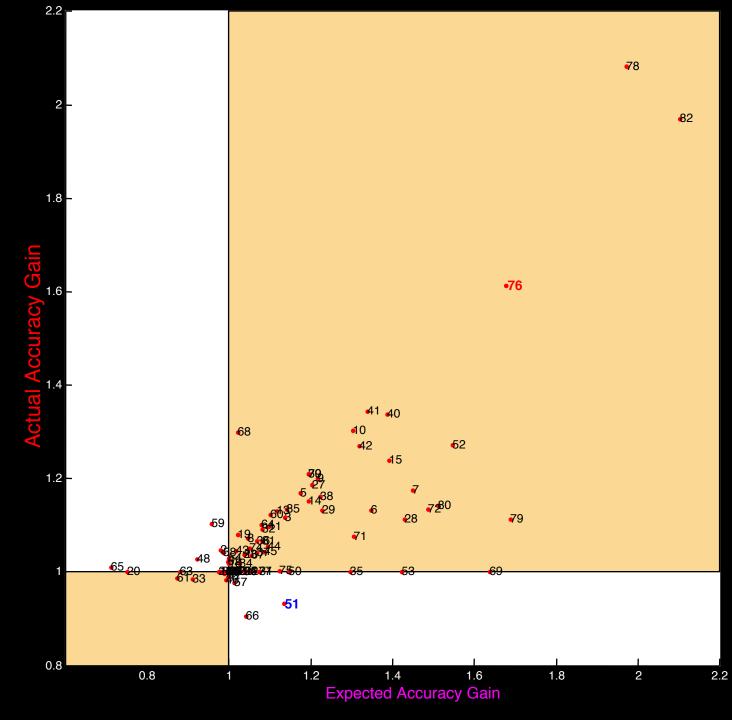
Expected Accuracy Gain

The results are strongly supportive of the claim "DTW better than Euclidean distance for most problems"

We sometimes had difficultly in predicting *when* DTW would be better/worse, but many of the training sets are tiny, making such tests very difficult.

For example, **51** is BeetleFy, with just 20 train and 20 test instances. Here we expected to do a little better, but we did a little worse.

In contrast, for **76** (LargeKitchenAppliances) we had 375 train and 375 test instances, and where able to more accurately predict a large improvement.



Recall the paper in SIGMOD that claimed "*Our STS3 approach is more accurate than DTW in our suitable scenarios*". And "*DTW outperforms STS3 in 79.5% cases.*" They are claiming to be better for 1/5th of the datasets, but in essence they are only reporting one axis of the Sharpshooter plot.

They did (slightly) win 20.5% of the time.

They lost 79.5% of the time.



*We had considered trying to reimplment this work to make this plot. But the idea has 3 parameters, and the writing is quite vague..

Recall the paper in SIGMOD that claimed "Our STS3 approach is more accurate than DTW in our suitable scenarios". And "DTW outperforms STS3 in 79.5% cases."

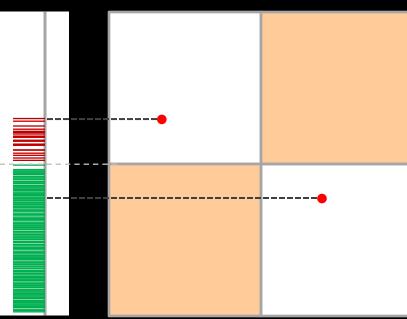
They are claiming to be better for 1/5th of the datasets, but in essence they are only reporting one axis of the Sharpshooter plot.

It may be^{*} that if we computed the Sharpshooter plot it would look like the below (for two selected points only)

They did (slightly) win 20.5% of the time, but they did not predict ahead of time that they would win.

They lost 79.5% of the time. Moreover, on a huge fraction of the datasets they lost on, they might have said "you should use our algorithm here, we think we will win", and we would have been much worse off!

*We had considered trying to reimplment this work to make this plot. But the idea has 3 parameters, and the writing is quite vague..



Expected Accuracy Gain

Summary for this section:

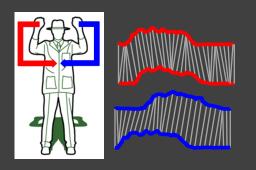
I think that at least 90% of the claims to beat DTW are wrong. Of the 10% of claims that remain

• They are beating the simplest 1NN-DTW with *w* learned in a simple way. Using KNN-DTW , smoothing the data, relaxing the endpoint constraints, better methods for learning *w* etc, would often close some or all the gap.

• The improvements are so small in most cases, it takes a sophisticated and sensitive test to be sure you have a real improvement.

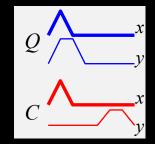
The Texas Sharpshooter test is a great sanity check for this, but you should see the work of Anthony Bagnall and students https://arxiv.org/abs/1602.01711 for a more principled methods.

Generalizing to Multi-Dimensional Data 1 of 4



It is increasingly common to encounter Multi-Dimensional (MD) time series data. Here we measure the X-axis acceleration of both the left and right hand.

Given these pair of 2D objects...



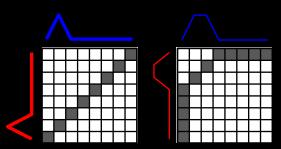
There are two obvious ways to compute the MD DTW score.

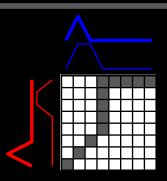
Independent: Just compute the DTW score for each dimension independently, and sum up each score.

 $DTW_{I}(Q,C) = DTW(Q_{x},C_{x}) + DTW(Q_{y},C_{y}) = 2.4$

Dependent: Create a single distance matrix that reflect the distance between each corresponding pair of time series, then find the *single* warping path and distance as per normal.

 $DTW_D(Q,C) = DTW(\{Q_x,Q_y\},\{C_x,C_y\}) = 3.2$





Generalizing to Multi-Dimensional Data 2 of 4

So, of DTW_1 and DTW_D which is best?

Lets think of it this way:

The thing we want classify is an physical process, the utterance of the word "*bicycle*", the beat of a heart, an autograph, a tennis shot etc.

We cannot see the actual event, just 2 or more time series it created.

–If the physical process affects the time series simultaneously, then DTW_{D} will probably be best. We call this the *tightly coupled* case.

–If the physical process affects the time series with varying lags, then DTW_I will probably be best. We call this the *loosely coupled* case.

Example: Suppose we measure the directionless acceleration of the left and right wrists of a tennis player.

The "physical process" is a *backhand stoke*. If a twohanded backstroke, the two time series are tightly coupled. If a one-handed backhand, the two hands will be very loosely coupled . Jo-Wilfried Tsonga



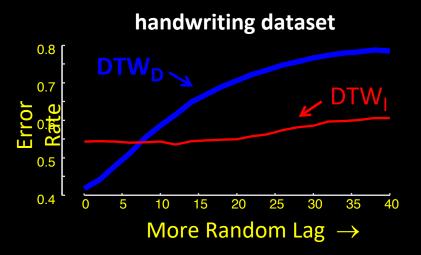
Generalizing to Multi-Dimensional Data 3 of 4

We can demonstrate the claim in the last slide with experiments.

Let us begin with a dataset that we are 100% sure is tightly coupled, then slowly add some random time lags into the data...

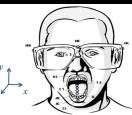
We know that the **handwriting dataset** is *tightly coupled*. We find that DTW_D has an error-rate of about 0.42, much better than that DTW_1 has an error-rate of about 0.55.

However, as we uncouple the perfect synchronization by adding some random lag, DTW_D quickly gets worse, while that DTW_I is barely effected.



Word Recognition from Articulatory Movement Data

Data	DTW(<u>1st</u>)	DTW(_{2nd})	DTW _I	DTW _D	
T1 _Z UL _X	0.34	0.59	0.25	0.31	У,
Τ1_Υ Τ1_Ζ	0.38	0.34	0.24	0.15	z 🖌



This effect is observed on real data

Note the results here show that..

- 1) Using 2D *can* be better than 1D
- 2) Noither DTM/ ner DTM/ deminater

Generalizing to Multi-Dimensional Data 4 of 4

Critical Point: You *can* generalize DTW to 2,3,4,...1,000 dimensions. However, it is *very* unlikely that more than 2 to 4 is useful, after that, you are almost certainly condemned to the curse of dimensionality.

Consider a physical activity dataset containing 36 axis synchronous measurements from three Inertial Measurement Units (IMUs) located on the wrist, chest and ankle. This dataset has eight subjects performing activities such as: rope-jumping, running, folding laundry, ascending-stairs.

Using *all* dimensions is a disaster! Using the best three is a lot better than using the best one, so there is evidence that Multi-Dimensional DTW really does help. PAMAP, Physical Activity Monitoring for Aging People www.pamap.org/ (we used DTW with *w* = 0 for simplicity here, we could do better by tuning *w*)



Which Dimensions?	Accuracy
All dimensions	0.19
A single random dimension (on average)	0.51
The best single dimension (as predicted by CV)	0.72
The best 3 dimensions (as predicted by CV)	0.89

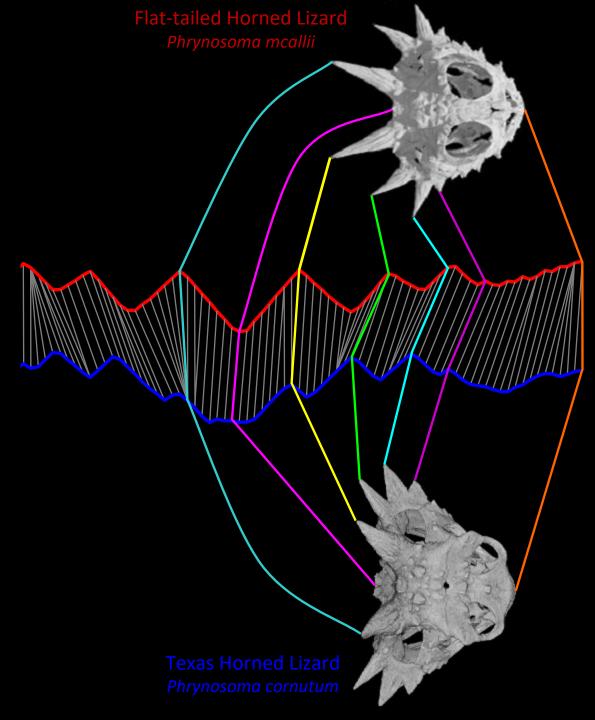


Summary...

DTW is an extraordinarily powerful and useful tool.

Its uses are limited only by our imaginations.

We believe it will remain and important part of the data mining toolbox for decades to come.



Coffee Break!

When we come back after the break

• Dr. Mueen will take over

 We will learn how to speed up DTW, and scale up to a trillion subsequences!



The Second Act: How to do DTW fast

- We are motivated that DTW is GOOD by the first act
- The general conception: *DTW is slow and we have a never-ending need for speed*
 - Better performance in knowledge extraction
 - Better scalability to process BigData
 - Better interactivity in human driven data analysis

What can be made fast?

One-to-One comparison

- Exact Implementation and Constraints
- Efficient Approximation
- Exploiting Sparsity

• One-to-Many comparisons

- Nearest Neighbor Search
 - In a database of independent time series
 - In subsequences of a long time series
- Density Estimation
 - In clustering
- Averaging Under Warping
 - In classification
- Many-to-Many comparisons
 - All-pair Distance Calculations

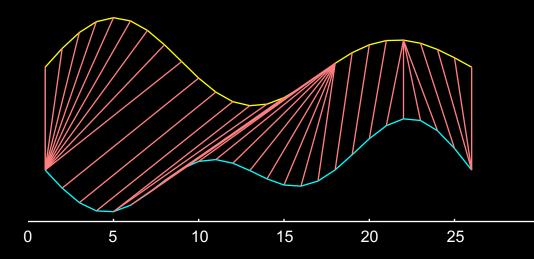
Speeding up DTW: one-to-one

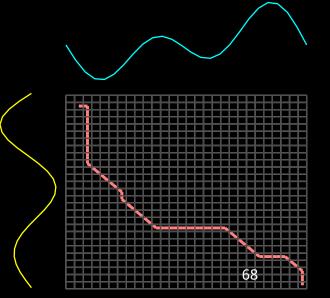
One-to-One comparison

- Exact Implementation
- Efficient Constraints
- Exploiting Hardware
- Efficient Approximation
- Exploiting Sparsity

Simplest Exact Implementation

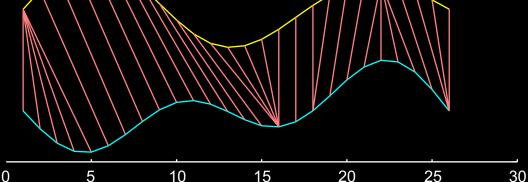
Input: x and y are time series of length n and m Output: DTW distance d between x and y D(1:n+1,1:m+1) = inf; D(1,1) = 0;for i = 2 : n+1 %for each row for j = 2 : m+1 %for each column $cost = (x(i-1)-y(j-1))^{2};$ D(i,j) = cost + min([D(i-1,j), D(i,j-1), D(i-1,j-1)]);d = sqrt(D(n+1,m+1));

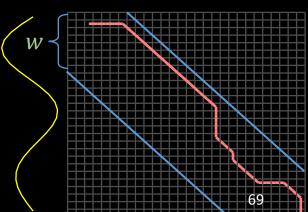




Simplest Implementation (Constrained)

```
D(1:n+1,1:m+1) = inf;
D(1,1) = 0;
w = max(w, abs(n-m));
for i = 2 : n+1
for j = max(2,i-w) : min(m+1,i+w)
cost = (x(i-1)-y(j-1))^2;
D(i,j) = cost + min( [ D(i-1,j), D(i,j-1), D(i-1,j-1) ]);
d = sqrt(D(n+1,m+1));6969
```

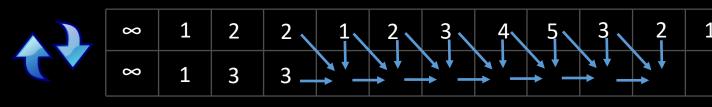




Memoization

```
D(2,1:m+1) = inf;
D(2,1) = inf;
D(1,1) = 0;
p = 1; c = 2;
for i = 2 : n+1
    for j = 2 : m+1
    cost = (x(i-1)-y(j-1))^2;
    D(c,j) = (x + min( [ D(p,j), D(c,j-1), D(p,j-1) ]);
    swap(c,p);
d = sqrt(D(n+1,m+1));
```

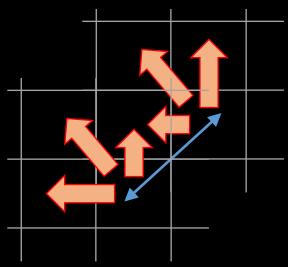
Previous Row



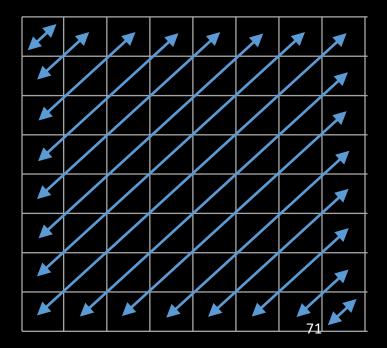
Current Row

Hardware Acceleration

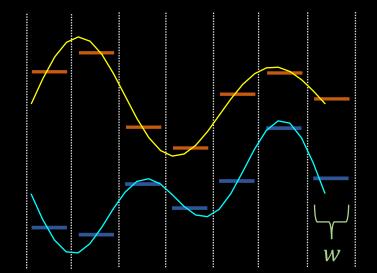
- Single Instruction Multiple Data (SIMD) architecture
- Cells on a diagonal are computed in parallel
- Values of a diagonal depend on the previous two diagonals

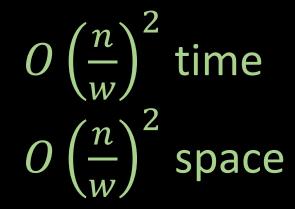


O(n) time O(n) space

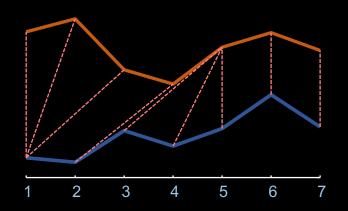


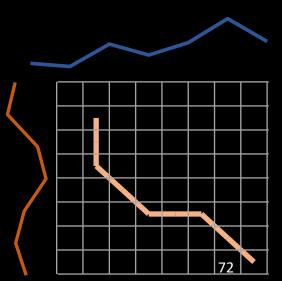
PAA based approximation





Piecewise Aggregate Approximation

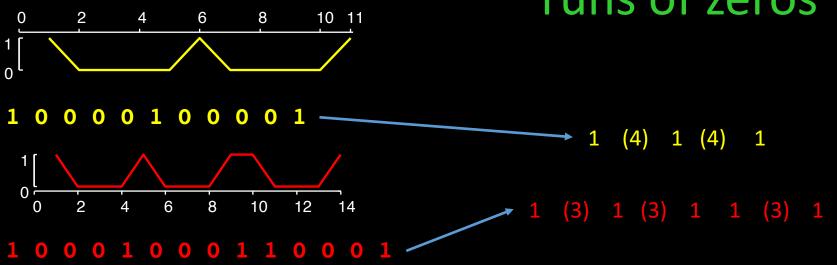




Selina Chu, Eamonn J. Keogh, David M. Hart, Michael J. Pazzani: Iterative Deepening Dynamic Time Warping for Time Series. SDM 2002: 195-212

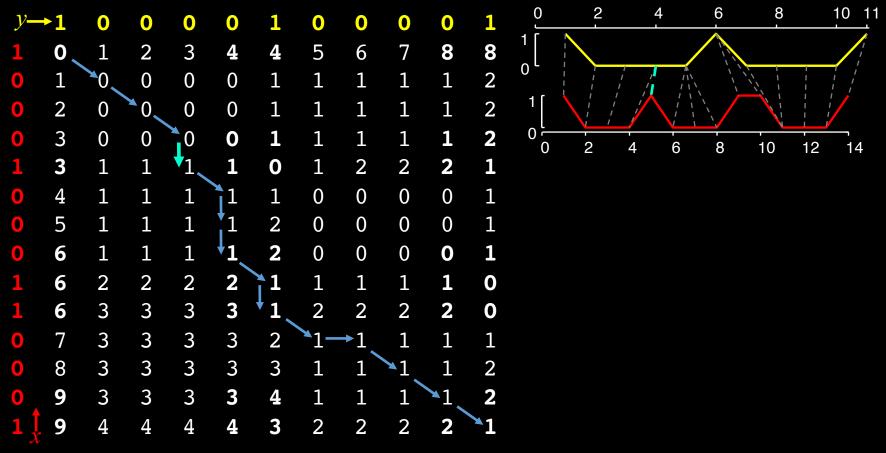
Approximation by Lengthencoding

To exploit sparsity, encode lengths of the runs of zeros

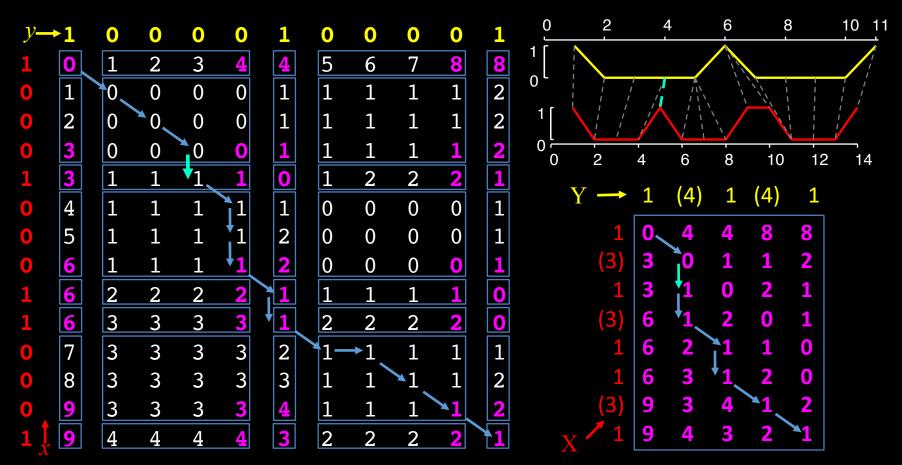


A Mueen, N Chavoshi, N Abu-El-Rub, H Hamooni, A Minnich, Fast Warping Distance for Sparse Time Series, Technical Report at UNM: 73 http://www.cs.unm.edu/~mueen/Projects/AWarp/awarp.pdf

Exploiting Sparsity (1)

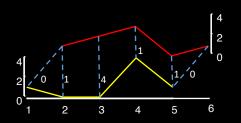


Exploiting Sparsity (2)

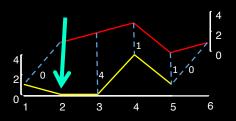


Exploiting Sparsity (2)

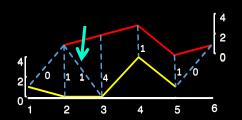
Correct Alignment



Missing Alignment



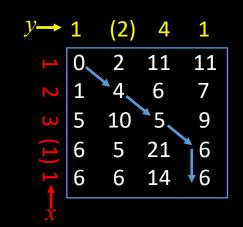
Extra Alignment



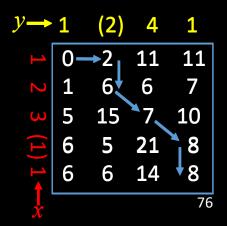
Non-Linear change → Exact Distance

0 $\mathbf{0}$ 11 \mathbf{O} 2 11 6 1 7 5 10 13 6 10 6 5 5 21 6 6 6 14 **√**7

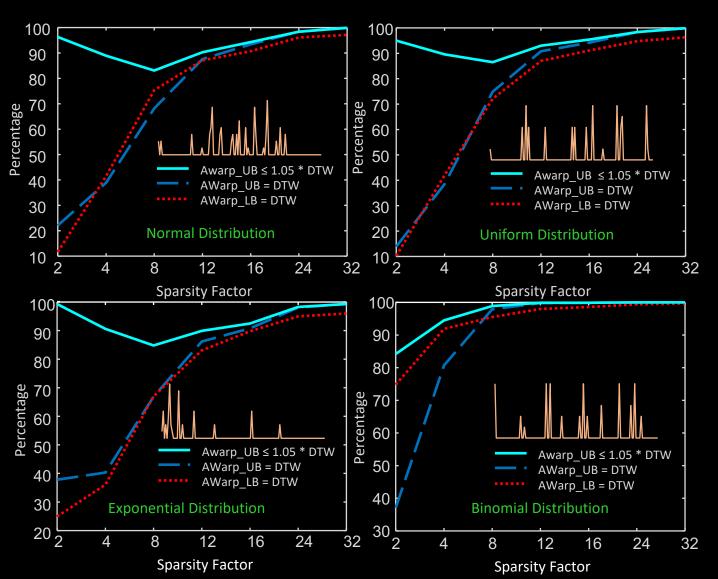
No change → Lower bound



Linear change → Upper bound



Exploiting Sparsity (3)



Sparsity Factor of *s* means $\frac{1}{s}$ % of the time series is filled with nonzeros.

What can be made fast?

- One-to-One comparison
 - Exact Implementation and Constraints
 - Efficient Approximation
 - Exploiting Sparsity
- One-to-Many comparisons
 - Nearest Neighbor Search
 - In a database of independent time series
 - In subsequences of a long time series
 - Density Estimation
 - In clustering
 - Averaging Under Warping
 - In classification
- Many-to-Many comparisons
 - All-pair Distance Calculations

Nearest Neighbor Search

- A query **Q** is given
- n independent candidate time series C₁, C₂, ..., C_n
- O(n) distance calculations are performed to

Find THE nearest neighbor of the given query under DTW.

Brute Force Nearest Neighbor Search

Computational cost: O(nm²)

Algo	Algorithm Sequential_Scan(Q)			
1.	<i>best_so_far</i> = infinity;			
2.	for all sequences in database			
3.				
4.				
5.	true_dist = DTW (C _i ,Q);			
6.	<pre>if true_dist < best_so_far</pre>			
7.	<pre>best_so_far = true_dist;</pre>			
8.	<pre>index_of_best_match=i;</pre>			
9.	endif			
10.				
11. endfor				

Lower Bounding Nearest Neighbor Search

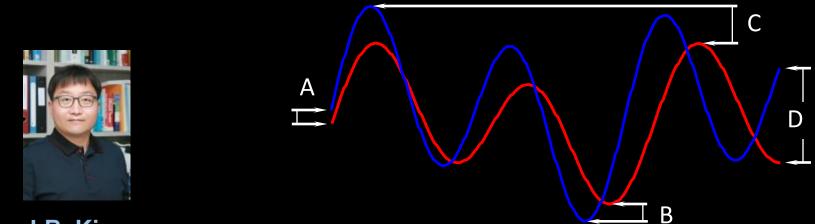
We can speed up similarity search under DTW by using a lower bounding function

Algorithm Lower_Bounding_Sequential_Scan(Q)		
1. <i>best_so_far</i> = infinity;		
2.	for all sequences in database	
3.	LB_dist = lower_bound_distance(C _i ,Q);	
4.	<pre>if LB_dist < best_so_far</pre>	
5.	true_dist = DTW (C _i ,Q);	
6.	<pre>if true_dist < best_so_far</pre>	
7.	<pre>best_so_far = true_dist;</pre>	
8.	<pre>index_of_best_match = i;</pre>	
9.	endif	
10.	endif	
11.	endfor	

Try to use a cheap lower bounding calculation as often as possible.

Only do the expensive, full calculations when it is absolutely necessary

Lower Bound of Kim



LB_Kim

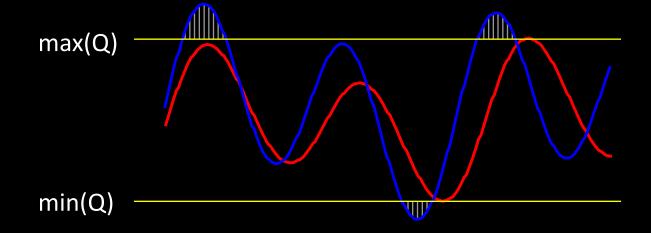
O(1) time if considered only first and last points O(n) time for all four distances

Kim, S, Park, S, & Chu, W. An index-based approach for similarity search supporting time warping in large sequence databases. ICDE 01, pp 607-614 The squared difference between the two sequence's first (A), last (D), minimum (B) and maximum points (C) is returned as the lower bound

Lower Bound of Yi

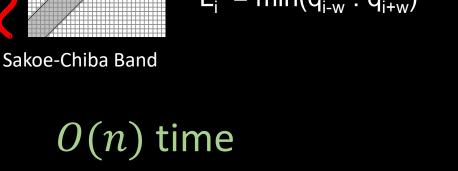


LB_Yi



O(n) time

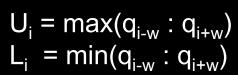
Yi, B, Jagadish, H & Faloutsos, C. *Efficient retrieval of similar time sequences under time warping*. ICDE 98, pp 23-27. The sum of the squared length of white lines represent the minimum contribution of the observations above and below the yellow lines.

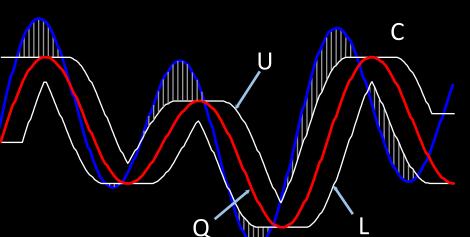


Envelope-Based Lower Bound

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





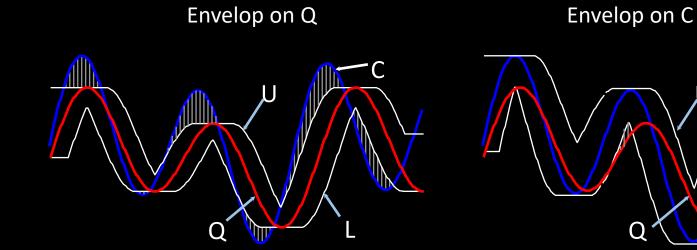


Q

U

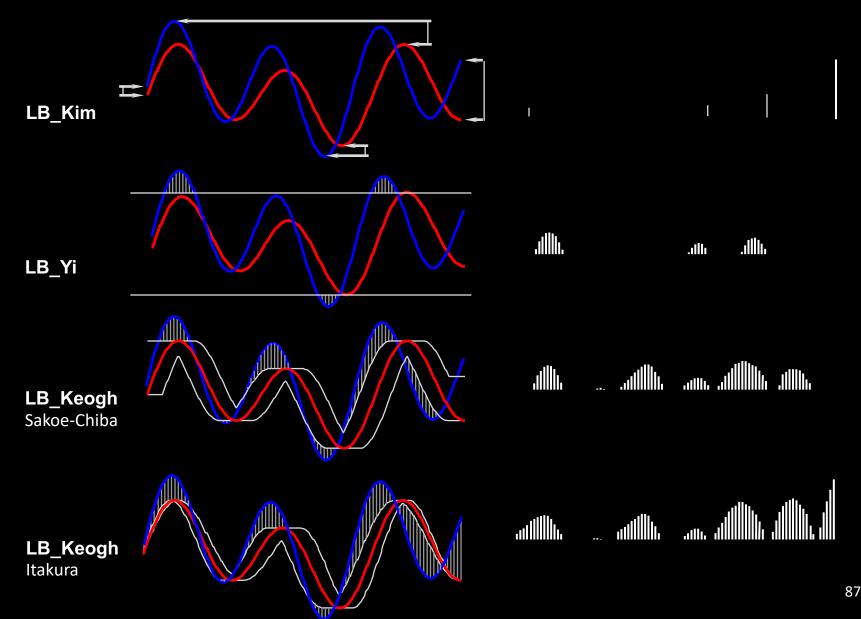
Reversing the Query/Data Role in LB_Keogh

- Make LB_Keogh tighter
- Much cheaper than DTW
- U/L envelops on the candidates can be calculated online or pre-calculated



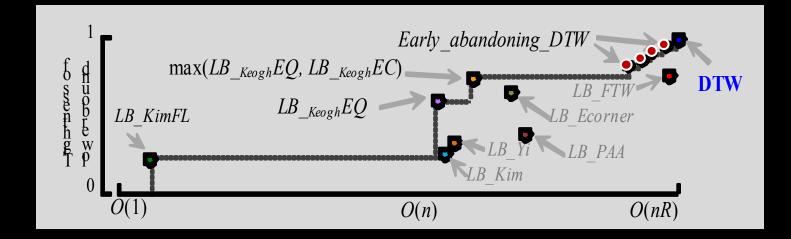


The tightness of the lower bound for each technique is proportional to the length of lines used in the illustrations



Cascading Lower Bounds

- At least 18 lower bounds of DTW was proposed.
- Use lower bounds only on the *Skyline*.
- Use the bounds on the skyline in cascade from least expensive to most expensive
- When unable to prune, use early abandoning techniques



99.9% of the time DTW is not calculated

Early Abandoning Techniques

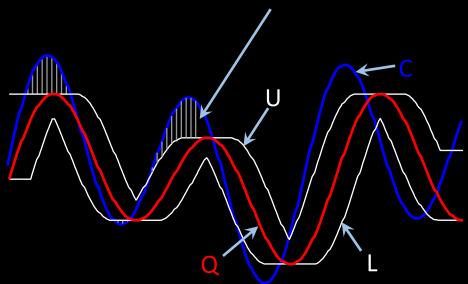
Abandon accumulating errors as soon as the current total is larger than the *best_so_far*

Four techniques to abandon early

- 1. Early Abandoning of LB_Keogh
- 2. Early Abandoning of DTW
- 3. Earlier Early Abandoning of DTW using LB_Keogh
- 4. Reordering Early Abandoning

Early Abandoning of LB_Keogh

Abandon the computation, when the accumulated error is larger than best_so_far

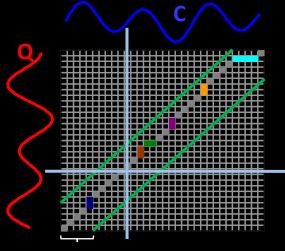


U, L are upper and lower envelopes of Q

Early Abandoning of DTW

dtw_dist

Abandon the computation, when the dtw_dist is larger than best_so_far

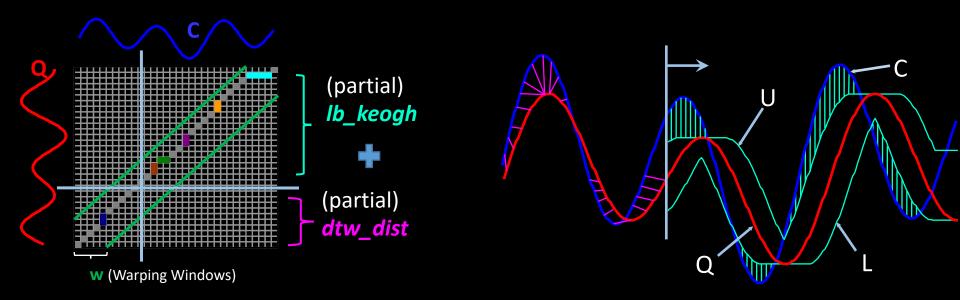


W (Warping Windows)

Q

Earlier Early Abandoning of DTW using LB_Keogh

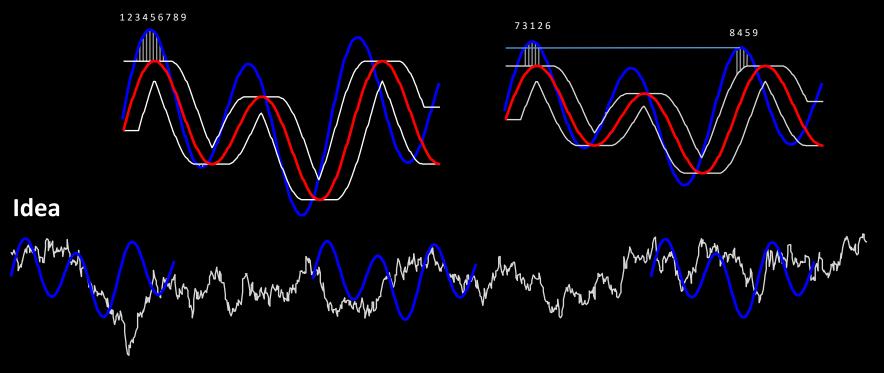
Abandon the computation, when the dtw_dist + lb_keogh is larger than best_so_far



U, L are upper and lower envelopes of Q

Reordering Early Abandoning

- We don't have to compute LB from left to right.
- Order points by expected contribution.



- Order by the absolute height of the query point.

Summary of the techniques

Group-1 Techniques

- Early Abandoning of LB_Keogh
- Early Abandoning of DTW
- Earlier Early Abandoning of DTW using LB_Keogh



Group-2 Techniques

- Just-in-time Z-normalizations
- Reordering Early Abandoning
- Reversing LB_Koegh
- Cascading Lower Bounds

UCR Suite Code and data is available at: www.cs.ucr.edu/~eamonn/UCRsuite.html

Thanawin Rakthanmanon, Bilson J. L. Campana, Abdullah Mueen, Gustavo E. A. P. A. Batista, M. Brandon Westover, Qiang Zhu, Jesin Zakaria, 94 Eamonn J. Keogh: Searching and mining trillions of time series subsequences under dynamic time warping. KDD 2012: 262-270

Experimental Result: Random Walk

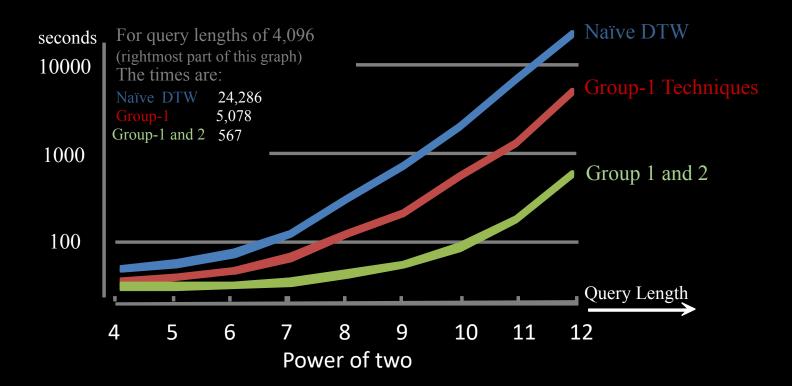
• Random Walk: Varying size of the data, |Q| = 128

	Million (Seconds)	Billion (<i>Minutes</i>)	Trillion (<i>Hours</i>)	Extrapolated
DTW-Naive	75.21	<u>1,252.2</u>	<u>20,869</u>	
Group-1	2.447	38.14	<u>472.80</u>	
Group-1 and 2	0.159	1.83	34.09	

- Experiments performed on a commodity machine
- Disk is accessed sequentially as the algorithm is invariant to data order
- The computation is performed while the next disk block is read

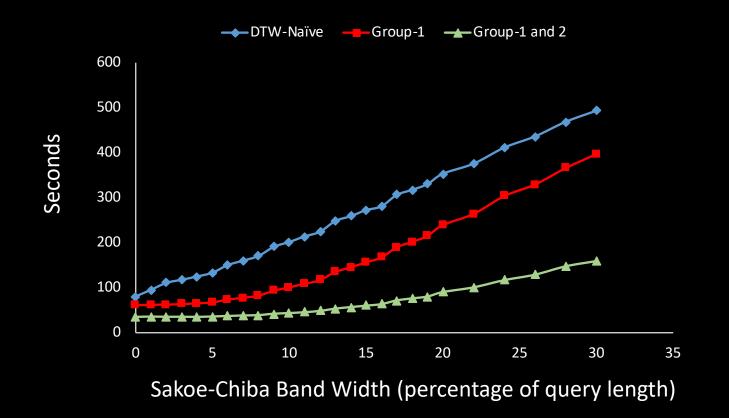
Experimental Result: Random Walk

• Random Walk: Varying size of the query, n = 20 million



Experimental Result: Random Walk

• Random Walk: Varying size of the band



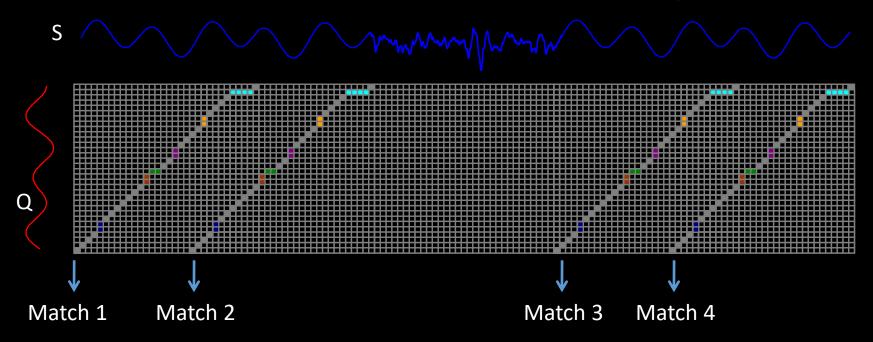
Nearest Subsequence Search

- A **Q** query is given
- A long time series of length n
- O(n) distance calculations are performed to

Find THE nearest subsequence of the given query under DTW.

Time Warping Subsequence Search

Reuses computation for subsequence matching



For every new observation only one column is added on the right

99

• No need for any of the techniques

Normalization is required

- If each window is normalized separately, reuse of computation is no longer possible
- To take advantage of the bounding and abandoning techniques, we need just-in-time normalization with constant overhead per comparison

Just-in-time Normalization

- In one pass, calculate cumulative sums of over x and x^2 and store $C = \sum x \qquad C^2 = \sum x^2$
- Subtract two cumulative sums to obtain the sum over a window $S_i = C_{i+w} - C_i$ $S_i^2 = C_{i+w}^2 - C_i^2$
- Use the sums to calculate the means and standard deviations of all windows in linear time

$$\mu_i = \frac{S_i}{w} \qquad \sigma_i = \sqrt{\frac{S_i^2}{w} - \left(\frac{S_i}{w}\right)^2}$$

 Dynamically normalize observations when calculating distance and possibly abandon early

$$cost = \left(\frac{x_{ij} - \mu_{xi}}{\sigma_{xi}} - \frac{q_i - \mu_{qi}}{\sigma_{qi}}\right)^2$$

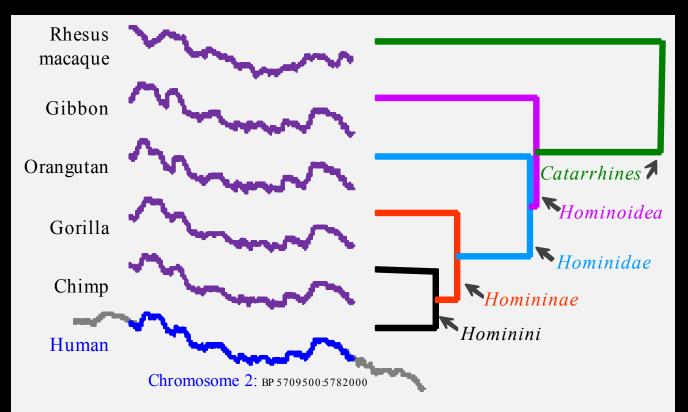
Experimental Result: ECG

- Data: One year of Electrocardiograms 8.5 billion data points.
- Query: Idealized Premature Ventricular Contraction (PVC) of length 421 (w=21=5%).
 PVC (aka. skipped beat)

	Group-1	Group 1 & 2
ECG	49.2 hours	18.0 minutes

Experimental Result: DNA

- Query: Human Chromosome 2 of length 72,500 bps
- Data: Chimp Genome 2.9 billion bps
- Time: UCR Suite 14.6 hours



What can be made fast?

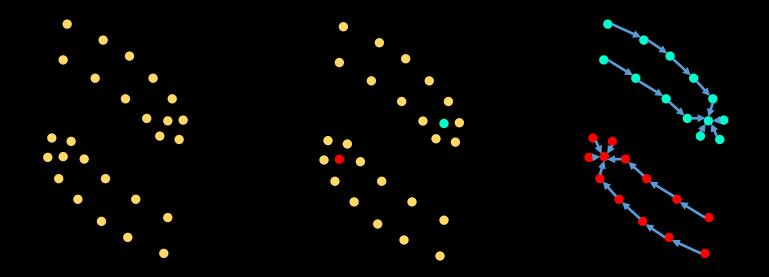
- One-to-One comparison
 - Exact Implementation and Constraints
 - Efficient Approximation
 - Exploiting Sparsity

One-to-Many comparisons

- Nearest Neighbor Search
 - In a database of independent time series
 - In subsequences of a long time series
- Density Estimation
 - In clustering
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- Many-to-Many comparisons
 - All-pair Distance Calculations

Density based clustering

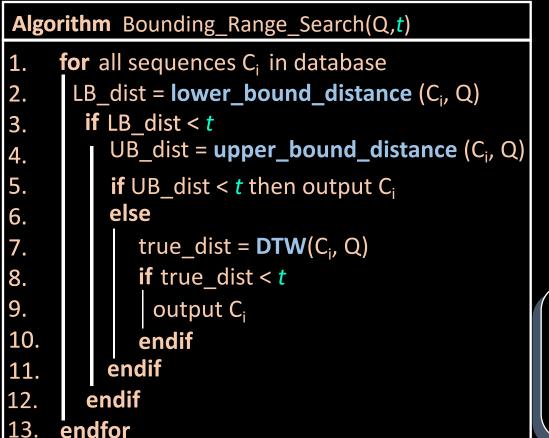
- Density Peaks (DP)* Algorithm
 - Find the densities of every point to pick cluster centers
 - Connect every point to the nearest higher density point

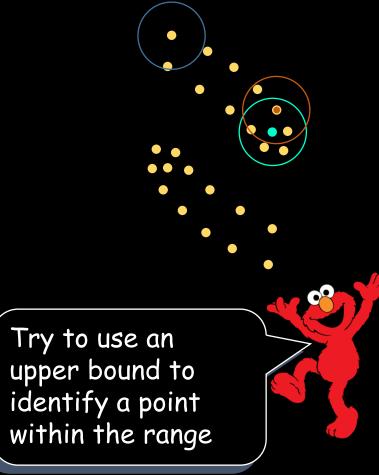


*Rodriguez, A., & Laio, A. (2014). *Clustering by fast search and find of density peaks*. *Science*, 344(6191), 149251496.

Range Search/Density Estimation

 Density is estimated by the number of points within a radius/threshold t

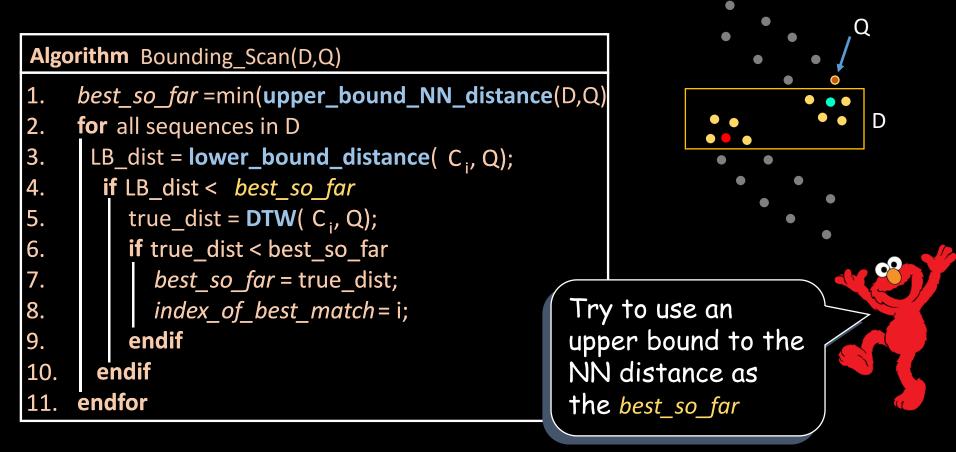




Nurjahan Begum, Liudmila Ulanova, Jun Wang, Eamonn J. Keogh: Accelerating Dynamic Time Warping Clustering with a Novel Admissible Pruning Strategy. KDD 2015: 49-58

Density Connectedness

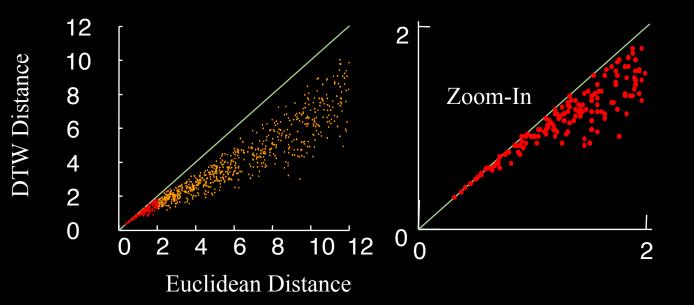
 Distance between a pair of points is an upper bound of the NN distance from both of the points

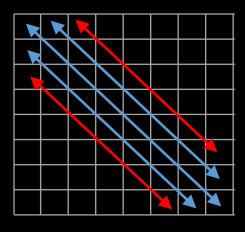


Nurjahan Begum, Liudmila Ulanova, Jun Wang, Eamonn J. Keogh: Accelerating Dynamic Time Warping Clustering with a Novel Admissible Pruning Strategy. KDD 2015: 49-58

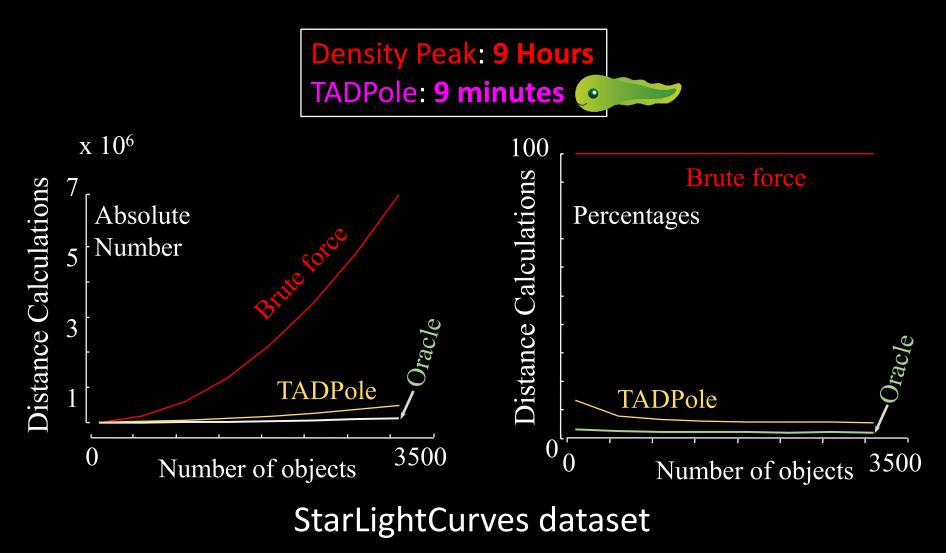
Upper bounding

- Euclidean distance is a trivial upper bound
- DTW distance in a band w is an upper bound for DTW distance in band w+1





Speedup by upper bounds



Nurjahan Begum, Liudmila Ulanova, Jun Wang, Eamonn J. Keogh: Accelerating Dynamic Time Warping Clustering with a Novel Admissible Pruning Strategy. KDD 2015: 49-58

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One-to-Many comparisons

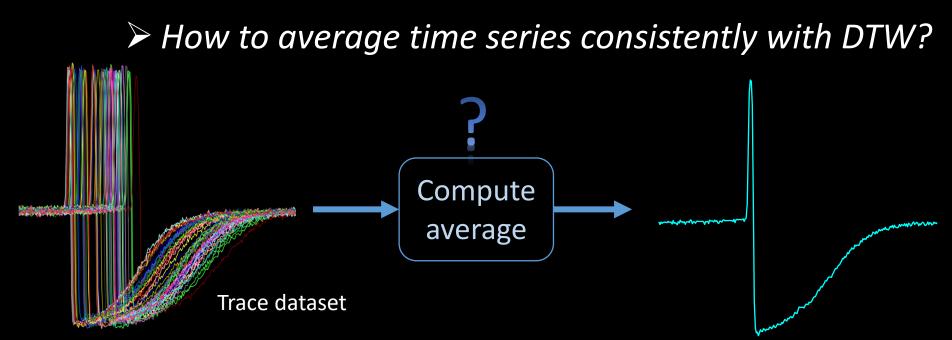
- Nearest Neighbor Search
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Data Reduction for 1NN Classification

- The training set is reduced to a smaller set keeping a representative set of labeled instances
- Smaller training set entails performance gain
- Smaller training set may gain accuracy if noisy instances are filtered effectively
- Reduction methods
 - Random Selection
 - Rank the instances and take top-K
 - Cluster instances based on proximity and take representative from each cluster

Many clustering algorithms require finding a centroid of two or more instances

The issue is then:

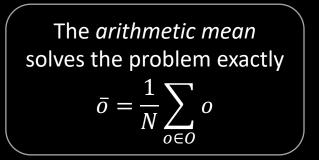


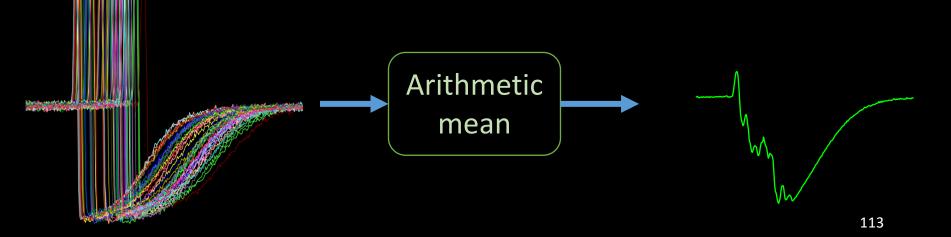
François Petitjean, Germain Forestier, Geoffrey I. Webb, Ann E. Nicholson, Yanping Chen, Eamonn J. Keogh: Dynamic Time Warping 112 Averaging of Time Series Allows Faster and More Accurate Classification. ICDM 2014: 470-479 Mathematically, the mean \overline{o} of a set of objects O embedded in a space induced by a distance d is:



The mean of a set minimizes the sum of the squared distances

If d is the Euclidean distance





To solve the optimization problem for DTW distance, we need to perform simultaneous alignment of many time series.

But, finding the optimal multiple alignment:

- 1. Is NP-complete [a]
- 2. Requires $O(L^N)$ operations
 - L is the length of the sequences (≈ 100)
 - N is the number of sequences (\approx 1,000)
- \Rightarrow Efficient solutions will be heuristic
- Pairwise Averaging
- DTW Barycenter Averaging (DBA)

[a] F. Petitjean, A. Ketterlin and P. Gançarski, "A global averaging method for dynamic time warping, with applications to clustering," *Pottern Recognition*, vol. 44, no. 3, pp. 678–693, 2011.

Pairwise averaging for DTW

- Average each alignment between the 0 two time series
- Commonly increases the length

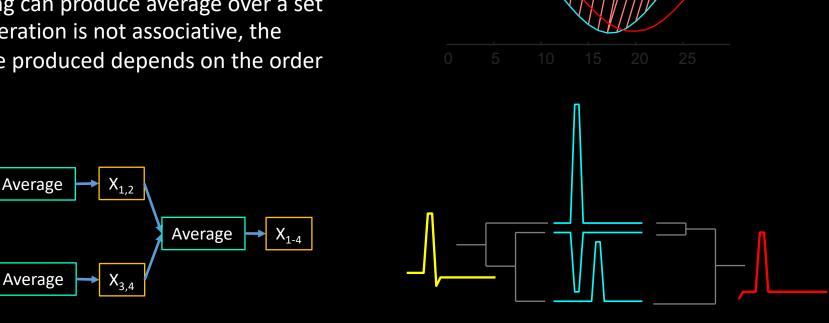
 X_1

 X_{2}

 X_3

 X_4

- Chaining can produce average over a set
- The operation is not associative, the • average produced depends on the order



Average

V. Niennattrakul and C. A. Ratanamahatana, "On Clustering Multimedia Time Series Data Using K-Means and Dynamic Time 115 Warping," IEEE International Conference on Multimedia and Ubiquitous Engineering, pp.733-738, 2007.

DTW Barycenter Averaging (DBA)

Algorithm DBA(D,av)

3

4

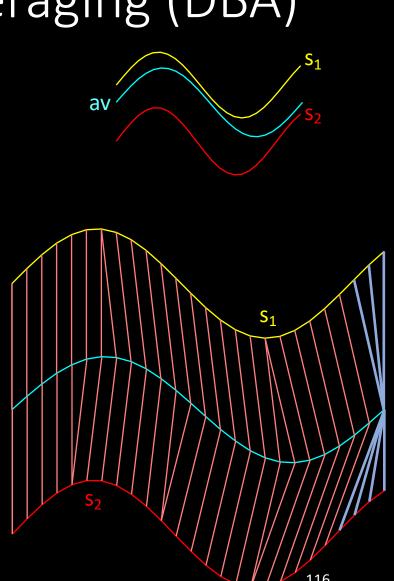
5

1 Iterate until convergence

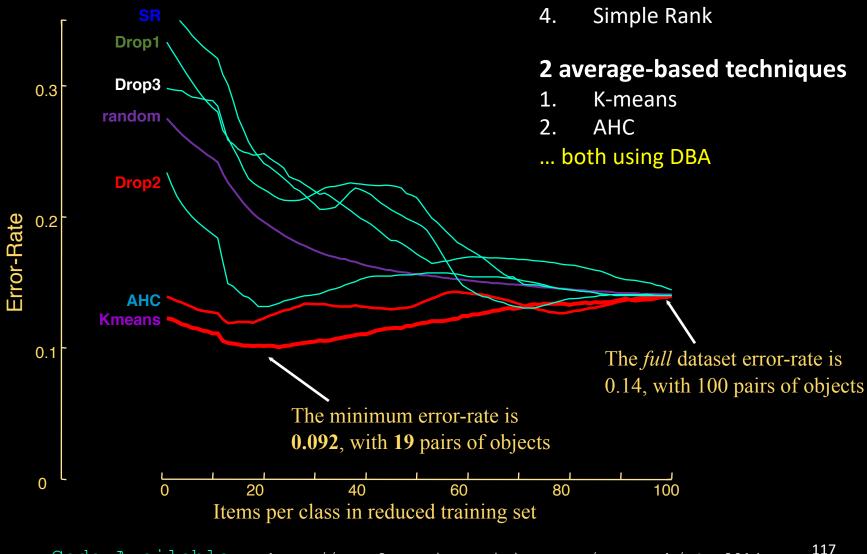
- 2 **for** each sequence s_i in D
 - A_i = GetAlignment(DTW(s_i, av))
 - **for** each observation *j* in av

 $av[j] = mean([A_1[j] A_2[j] A_3[j] A_n[j])$

- Does not increase length
- Does not depend on the order of the points



Experimental Evaluation on Insect Data



Code Available : http://www.francois-petitjean.com/Research/ICDM2014-DTW

4 rank-based competitors

1. Drop 1

2.

3.

Drop 2

Drop 3

What can be made fast?

- One-to-One comparison
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 - Exploiting Sparsity
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Speeding up DTW: many-to-many

- Several variants
 - Self-join within a threshold top-K Self-join
 - Use similarity search techniques as subroutine
 - Application: Motif discovery [a], Discord discovery
 - A/B Join within a threshold top-K A/B Join
 - Use similarity search techniques as subroutine
 - Application: Motion Stitching [b]
 - All-pair distance matrix
 - Use techniques to speedup one-to-one comparisons
 - Application: Hierarchical Clustering

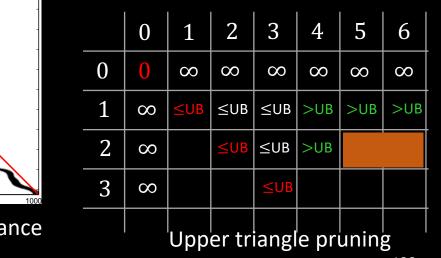
[a] N Chavoshi, H Hamooni, A Mueen, "DeBot: Real-Time Bot Detection via Activity Correlation" UNM Technical Report
 [b] Y. Chen, G. Chen, K. Chen and B. C. Ooi, "Efficient Processing of Warping Time Series Join of Motion Capture Data," ICDE, 2009, pp. 1048-1059.

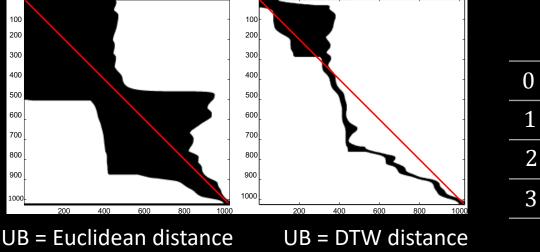
PrunedDTW: speeding up all-pair distance matrix calculation

- Two types of pruning when calculating DTW matrix
- Exact method



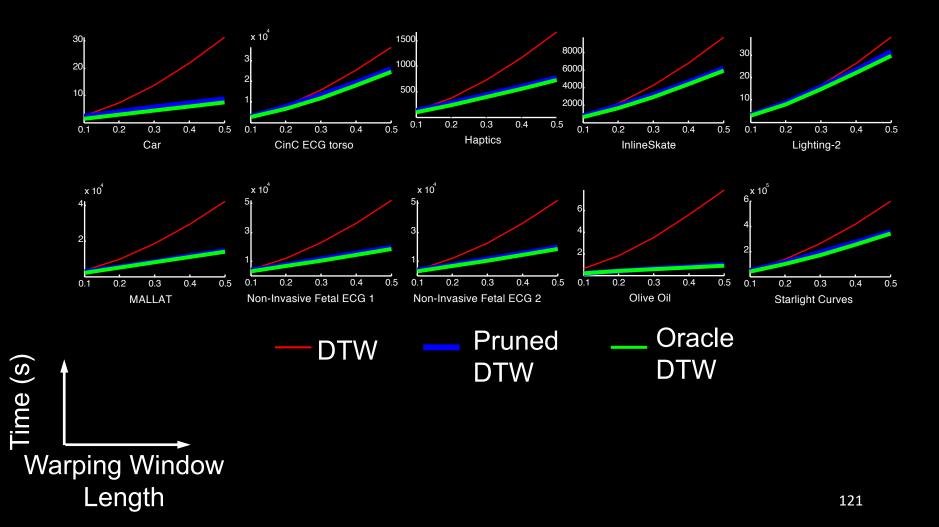
Lower triangle pruning





Diego F. Silva, Gustavo E. A. P. A. Batista, Speeding Up All-Pairwise Dynamic Time Warping Matrix Calculation, SDM 2016

Experiments



Conclusion

- Nearest neighbor search under warping is fast enough for most practical purposes
- Data reduction improves 1NN classification both in speed and accuracy
- DTW is an extraordinarily powerful and useful tool. Its uses are limited only by our imagination.



Additional References

- H. Sakoe and S. Chiba, "Dynamic programming algorithm optimization for spoken word recognition," IEEE Trans. Acoust. Speech, Lang. Process., vol. 26, no. 1, pp. 43–50, 1978.
- Mustafa S. Çetin, Abdullah Mueen, Vince D. Calhoun: Shapelet Ensemble for Multi-dimensional Time Series. SDM 2015: 307-315
- X. Wang, A. Mueen, H. Ding, G. Trajcevski, P. Scheuermann, and E. Keogh, "Experimental comparison of representation methods and distance measures for time series data," Data Min. Knowl. Discov., vol. 26, no. 2, pp. 275–309, 2013.
- D. Sart, A. Mueen, W. Najjar, V. Niennattrakul, and E. Keogh, "Accelerating Dynamic Time Warping Subsequnce Search with GPUs and FPGAs. ICDM 2010," in Proceedings - IEEE International Conference on Data Mining, ICDM, 2010, pp. 1001–1006.
- Abdullah Mueen, Hossein Hamooni, Trilce Estrada: Time Series Join on Subsequence Correlation. ICDM 2014: 450-459
- Ira Assent, Marc Wichterich, Ralph Krieger, Hardy Kremer, and Thomas Seidl. 2009. Anticipatory DTW for efficient similarity search in time series databases. Proc. VLDB Endow. 2, 1 (August 2009), 826-837.