

cuTimeWarp: Accelerating Soft Dynamic Time Warping on GPU

Alex Kylo

Afrooz Rahmati

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Abstract

This report explores techniques for optimizing the computation of Soft Dynamic Time Warping, a differentiable sequence dissimilarity measure, on graphics processing units (GPU), for the purpose of enabling high-performance machine learning on time series datasets.

Introduction

Time series machine learning is a research area with countless useful applications such as recognizing sounds and gestures. Clustering or classifying large time series datasets is challenging partly because of the need to define a measure of dissimilarity between any two given time series. Furthermore, practical applications require finding common structure in time series despite different speeds or phases; for example, a word means the same whether spoken quickly or slowly. Another requirement for machine learning tasks is that the dissimilarity measure must be differentiable so that its gradient can be used as to minimize it as a loss function to find the best fit model. Finally, the measure must be efficient to calculate, because it will be calculated repeatedly many times during model fitting. To this end we will explore GPU acceleration of Soft Dynamic Time Warping (Soft-DTW) [1], a differentiable sequence dissimilarity measure, to enable high performance time series machine learning.

Background

TODO: add an intuitive explanation of what time series data is The purpose of dynamic Time wrapping (DTW) is to perform a transformation function that wrap the time to align two time series. Preferably we tend this alignment to be optimum and satisfy our requirements.[2]

DTW is a widely used tool employed in many areas of science, including biology, technology, economics, and finance. It calculates the practical distance between two signals typically by taking the distance between them when one is time warped, or it can be the minimum wrapping required to align signals with each other by applying some sort of fidelity. Dynamic time wrapping can be used to identify hidden pattern or searching within signals databases to find the matching one.[3] it is utilized in machine learning platforms that depends on signals like clustering, regression, and classification.

There are multiple valid ways to compute a measure of dissimilarity between two time series; the simplest is Euclidean distance, which is the square root of the sum of squared pairwise differences between two time series x and y , each of length n (equation 1).

$$d(x, y) = \sqrt{\sum_{t=1}^n (x_t - y_t)^2} \quad (1)$$

The drawback of Euclidean distance in time series applications is that two structurally similar time series will produce a large distance if they are different speeds or out of phase (TODO: Add a figure to illustrate this).

Dynamic Time Warping (DTW) was devised in the 1960s as an alternative time series dissimilarity measure to address this shortcoming. (TODO: find a historical citation). DTW is a nonlinear mapping of from each point in one time series to the nearest point in a second time series. While DTW is technically not considered a “distance” because it does not conform to the triangle inequality, and therefore we refer to it as a “dissimilarity” instead, it can be used in place of Euclidean distance or other distance measures for many applications of time series data.

The basic algorithm for DTW is to use Bellman’s recursion, a dynamic programming technique, to find the lowest-cost path diagonally across a pairwise distance matrix. The computation cost for this approach is quadratic ($O(mn)$) for time series vectors of length m and n [1]. The formula for the DTW between time series x and y is given by equation 2. (TODO: explain the algorithm in more detail and provide a visualization)

$$DTW(x, y) = \min_{\pi} \sqrt{\sum_{(i,j) \in \pi} d(x_i, y_j)^2} \quad (2)$$

Where $d(x_i, y_j)^2$ is the cost function, typically pairwise squared Euclidean distance. The loss function for DTW is not differentiable due to the min operation within the formula; a small change in the input time series may result in zero change in the path cost. However, we can create a differentiable version called Soft-DTW by replacing the min function with a soft-min function (equation 3) [1].

$$\text{soft-min}_{\gamma}(a_1, \dots, a_n) = -\gamma \log \sum_i e^{-a_i/\gamma} \quad (3)$$

Hence, Soft-DTW is parameterized by the smoothing constant gamma, which becomes a tunable hyperparameter in machine learning model training applications.

A common technique in machine learning with Soft-DTW is the computation of barycenters, which are centroids within the space of a set of time series. The differentiability of Soft-DTW allows for barycenter finding via gradient descent, and then new observations can be classified by finding the nearest barycenter. Sequence prediction and generation of is also possible using recurrent neural networks with Soft-DTW as a loss function [1].

(TODO: Explain process of barycenter finding with gradient descent on softdtw loss)

Prior to computing the Soft-DTW dissimilarity between any two time series, each time series should be *z-normalized*, that is, scaled so that its mean is equal to 0 and its standard deviation is equal to 1, to remove the problem of “wandering baselines” or “drift” in the measurements, as illustrated in [4] with an ECG classifier that yields incorrect results on un-normalized data due to drift that “may be caused by patient movement, dirty lead wires/electrodes, loose electrodes, and so on,” and which “does not have any medical significance.” Z-normalization also tends to make the iterative process of minimizing the cost function through gradient descent or quasi-Newtonian methods more efficient because its hyperplane is not disproportionately stretched in any one dimension, so the step size in any direction is the same relative to the scale of that dimension. (TODO: explain this better, find a citation)

Related Work

Utilizing indexing to construct lower bounds on warping distance is an optimization technique for speeding up nearest neighbor search via early removal of poor candidates [5]. Shen and Chi (2021) proposes an optimization of nearest neighbor search of multivariate time series, leveraging the triangle inequality and quantization-based point clustering to restrict the search [6].

Xiao et al (2013) introduced a prefix computation technique for transforming the diagonal data dependence to improve parallel computation of the cost matrix on GPU [7]. Zhu et al (2018) demonstrates a method of optimizing memory access by taking advantage of the diagonal data dependency to rearrange the matrix so that elements on the same diagonal are stored contiguously [8]. A prior implementation of Soft-DTW on CUDA using PyTorch and Numba is capable of 100x performance improvement over the original Soft-DTW Cython code, but is limited to sequence lengths of 1024 (CUDA max block size) and leaves many opportunities for further CUDA optimizations such as the use of shared memory [9]. A 2015 paper describes a tiling approach called *PeerWave*, which utilizes direct synchronization between neighboring streaming multiprocessors (SMs) to handle the inter-tile data dependency without atomic operations, locks, or other global barriers, leading to improved load balance and scaling properties [10].

In our project we will focus on this area of opportunity, optimizing matrix structure and memory access patterns to maximize parallelism and minimize memory latency in the computation of the warping path matrix.

Methods

To evaluate various performance optimizations on the Soft-DTW computation, we implemented a C++ and CUDA library called *cuTimeWarp*, which includes functions for computing the SoftDTW on CPU and GPU.

Given a set of many multivariate time series of the same length and number of variables, we can compute the Soft-DTW distance between every time series and every other time series in the set by computing, in parallel for each pair, a pairwise squared Euclidian matrix, then applying the Soft-DTW calculation on the distance matrix. This computation, however, also has an $O(n^2)$ complexity and can potentially take longer than the DTW computation itself. For univariate time series, we can save this cost by compute the DTW cost matrix on the two input time series directly, computing the absolute distance between each pair of values from the two time series within the nested loop of the DTW procedure.

Optimization Techniques

Shared memory stencil computation

As the program iterates diagonally across the distance matrix to find the optimal warping path, each cell in the path utilizes the previously computed results of three previous neighboring cells; if the iteration is visualized as proceeding from the upper left to the lower right corner of the matrix, the cost value in each cell depends on the (soft) minimum of the costs in the cell above, the cell to the left, and the cell to the diagonal upper-left, which were computed in the previous two iterations (Figure 1). If the cost matrix R resides in global memory, then non-contiguous accesses to $R[i-1][j]$, $R[i][j-1]$ and $R[i-1][j-1]$ will result in cache misses, incurring a significant performance cost. Since each element of R will be referenced up to three times in the computation of dependent cells, these cache misses can be avoided via a stencil computation using shared memory in CUDA. The stencil serves as a cache for the current and previous two diagonals; once a diagonal is no longer in use, its elements are written back to the cost matrix R in device global memory.

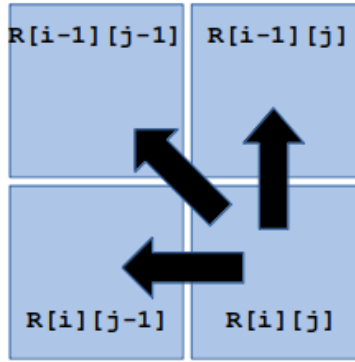


Figure 1: Data dependency direction between cells of the cost matrix

The algorithm can be modified to use shared memory as follows:

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D is a squared euclidean distance matrix of two time series
R is a cost matrix initialized to positive infinity except for  $R[0, 0] = 0$ 
for each anti-diagonal of R starting from  $R[0, 0]$ 
    if the current thread index < length of the current anti-diagonal
        copy  $R[i][j]$  from global memory into the stencil array
        read  $R[i-1][j]$ ,  $R[i][j-1]$  and  $R[i-1][j-1]$  from the stencil array
        compute cost as  $\text{softmin}(R[i-1][j], R[i][j-1], R[i-1][j-1]) + D[i-1][j-1]$ 
        write the cost back to the stencil
        copy the cost in  $R[i-1][j-1]$  from the stencil back to global memory

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Sakoe-Chiba bands

Sakoe-Chiba bands, proposed by Sakoe and Chiba in their 1978 paper "Dynamic programming algorithm optimization for spoken word recognition," introduce a "slope constraint" to the warping path to limit the maximum allowed warping distance beyond which a pair will not be considered in the optimal path calculation [11]. Pruning the search space by removing some of the extreme diagonals from consideration yields an approximation of the optimal warping path that can be calculated in sub-quadratic time.

This optimization is simple to implement for square matrices (i.e. DTW on time series of equal length) by checking that the absolute difference between the loop counter variables i and j does not exceed a fixed bandwidth threshold value (Figure 2). For rectangular matrices, since the leading diagonal does not end at the lower right corner, the implementation must be modified slightly to ensure that the counter variable along the longer of the two dimensions stays within a defined radius.

In a parallel programming environment such as CUDA, this optimization can also allow for the computation of the warping path using fewer threads, as threads assigned to cost matrix cells outside the band would go unused.

While this technique produces only an approximation of the optimal path, in practice it has been shown to improve task performance by preventing pathological alignments where a very small portion of one time series maps onto a large portion of the other [5]. The width of the band can be a tunable hyperparameter for time series classification tasks.

Test Data

For performance testing we selected datasets from the UCR Time Series Archive [12] and the UEA Multivariate Time Series Classification Archive [13].

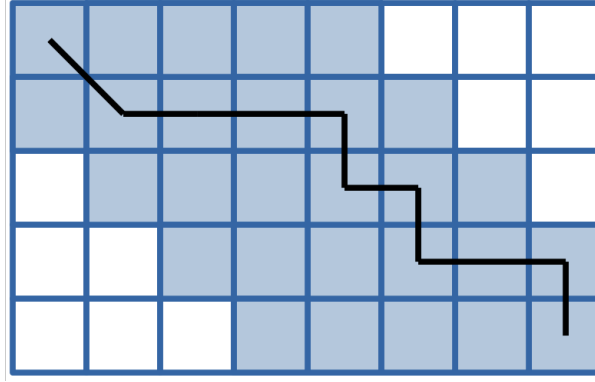


Figure 2: Illustration of an optimal DTW path through a 5x8 distance matrix with radius = 1

Results

Discussion

Future Work

Our library provides CUDA kernels and C++ wrappers for computing pairwise Soft-DTW dissimilarity measures as well their gradients in parallel. Potential future work includes integrating this library with an optimization library that can iteratively minimize Soft-DTW cost to find barycenters among a set of time series, to assemble a nearest centroid classification system. Another area of potential is writing Python bindings to expose the Soft-DTW loss and gradient functions to deep learning frameworks such as TensorFlow or PyTorch, to enable the use of Soft-DTW loss as a training objective for recurrent neural networks. This will facilitate tasks such as classifying, predicting and generating sounds, gestures, and sensor data under the dynamic time warping geometry.

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