

Chapter 1

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Leveraging Nearest Neighbors for Time Series Forecasting with Matrix Profile

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1.1 Background

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Humans have made predictions since ancient times. In ancient societies, accurate predictions were important to the success of subsistence activities such as hunting, planting, and harvesting. There was a need to predict weather dynamics, such as rainfall and temperature. For example, it is crucial to plant during the period with sufficient rainfall and appropriate temperatures. Our ancestors used divination tools such as turtle shells, wooden blocks (moon blocks), or bones to make predictions. Without doubt, the accuracy was not guaranteed. Even in modern societies, prediction is still essential. Predicting traffic-jam patterns only a few hours ahead can save time by enabling the selection of an alternative route [1]. A wealth could be created by forecasting stock market trends. Predicting the future, also known as time series forecasting, is crucial.

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With advances in hardware technologies, we collect enormous amounts of data from diverse sources, such as smart sensors and social media platforms, continuously in the form of time series data. A time series is an ordered sequence of measures, represented in real-valued numbers, at discrete equal-interval timestamps [2]. The vast data collections have created the era of “Big Data”, which provides a wealth of datasets for developing and deploying reliable, robust, data-driven forecasting techniques to discover patterns and extract valuable information [3]. Applications can be found in the financial sector, such as predicting

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25 business cycles and stock market movements [4, 1, 5, 6] and the medical field,
 26 such as the status of critical patients according to their vital signs [7, 8] and the
 27 propagation of diseases such as influenza [6, 9] and COVID-19 [7, 10].

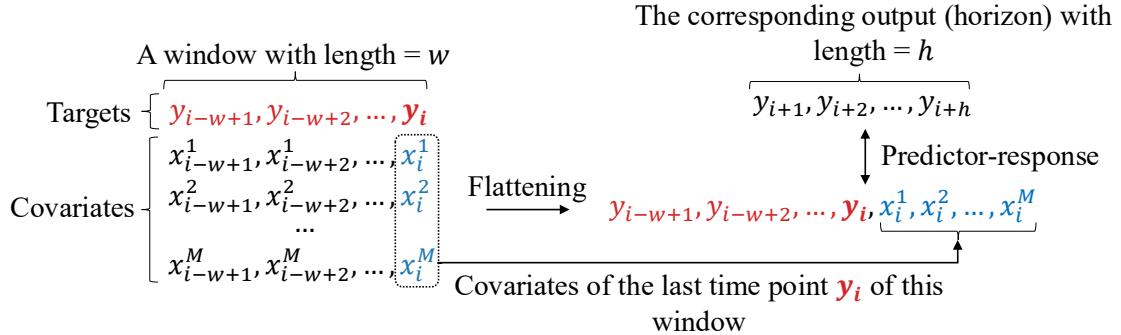


Figure 1.1: Flattening a 2D window of size $(1 + M) \times w$ to a 1D vector of length $w + M$. The resulting vector serves as the *predictor* for the regressor. Its expected *response* is the vector of length h . The regressor learns from this predictor-response pair.

28 A recent study [11] shows that, in time series classification, a non-parametric,
 29 instance-based method, namely nearest-neighbor classifiers (1-NN) and its gen-
 30 eralized form k -NN, with appropriate distance measures, such as Dynamic Time
 31 Warping (DTW), despite their simplicity, perform well and are therefore com-
 32 monly used as benchmarks. In detail, when a new instance is to be classified,
 33 k -NN finds its k nearest neighbors in the training set and returns their majority
 34 label among them. k -NN is considered a lazy learner because the training steps
 35 involve only memorizing all the instances verbatim; no higher-level concepts have
 36 been learned. In addition, in time series forecasting, a recent study demonstrates
 37 that a well-known machine learning baseline, Gradient Boosting Regression Tree
 38 (GBRT), such as XGBoost, equipped with an appropriate data engineering of the
 39 data, can achieve competitive or even superior performance than the deep learning
 40 method. In detail, they transform the time series forecasting task into a window-
 41 based regression problem, as shown in Figure 1.1. For each training window of
 42 length w with the last time point \mathbf{y}_i , and its lagged values $\mathbf{y}_{i-1}, \mathbf{y}_{i-2}, \dots, \mathbf{y}_{i-w+1}$ are
 43 concatenated with covariates $x_i^1, x_i^2, \dots, x_i^M$ to form a *predictor* for a multi-output
 44 GBRT. This transformation is called flattening. The corresponding response is the
 45 following h points of \mathbf{y}_i . It provides a simple, more efficient yet accurate method
 46 for time series forecasting.

47 Moreover, k -NN has also shown to be a promising method for time series fore-
 48 casting [12]. The k -NN uses the lagged values of the last time point to form a
 49 query Q . It identifies the k previous similar subsequences to Q and uses their

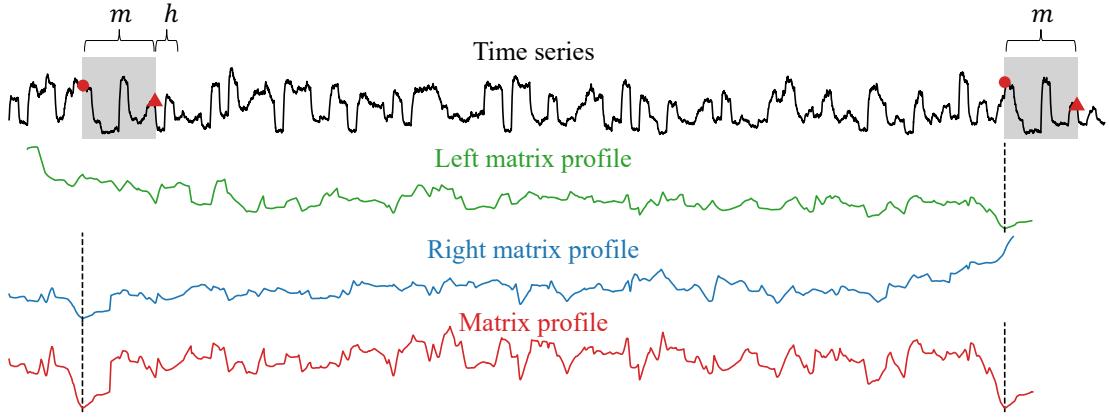


Figure 1.2: The **left** (**right**) matrix profile and the **matrix profile** of a time series. The **matrix profile** shows the distances between each m -subsequence and its nearest neighbor, where m is a user-given value. The **left** (**right**) matrix profile shows the same information but is limited to its left (right) nearest neighbor. For a particular m -subsequence shown by the right gray box, its nearest neighbor is the left gray box, as indicated by the dashed line in the **left matrix profile** and the **matrix profile**. Similarly, the nearest neighbor of the left gray box is the right gray box, as indicated by the dashed line in the **right matrix profile** and the **matrix profile**. The first (last) point in each box is denoted by a red circle (triangle). h denotes the length of the immediate subsequence of the nearest neighbor. Intuitively, this subsequence should be similar to the immediate subsequence (i.e., future) of the right gray box. To note, the **left** (**right**) matrix profile starts (ends) at a later (earlier) index because the corresponding nearest neighbor with length m does not exist.

Algorithm 1 The brute force approach to compute Matrix Profile

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1: for  $i \leftarrow 1$  to  $n - m + 1$  do
2:   for  $j \leftarrow 1$  to  $n - m + 1$  do
3:     Compute the z-normalized Euclidean distance between  $t_{i,m}$  and  $t_{j,m}$ .

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immediate subsequences to predict the immediate subsequence, which is the forecasting window, of Q . The intuition is that history repeats itself. The previous (historical) subsequences that are similar to Q can provide a hint about the future of Q . They are similar, and so are their immediate subsequences. Figure 1.2 depicts this idea. Observe that the immediate subsequence of the right gray box is similar to that of the left gray box. The left gray box is the nearest neighbor of the right gray in the “past”.

Based on these findings, this study proposes a method to improve the performance of existing forecasters by leveraging information from the nearest neighbors of each subsequence in the target variable. For each time point y_i of the target variable Y , a window of length w is constructed with y_i as the last point, then

we retrieve the window’s historical nearest neighbors and use their information to create new covariates for the window. The information includes the similarities between the window and its nearest neighbors, as well as the immediate subsequences of them. The similarity can be interpreted as a measure of confidence or weight in using the information from the corresponding nearest neighbor. The intuition is that, if the similarity of the window and a neighbor is high, then the future (i.e., immediate subsequence) of the neighbor should also be similar to the future of the window. The fundamental difference between this study and previous approaches [13, 12, 14] is that they directly use the subsequent points for prediction, whereas we use the nearest neighbor information for each subsequence as covariates, which are used as primitives for other forecasters. We explain this subtle difference by Figure 1.2. The previous approaches simply use the information of the nearest neighbors of the last look-back window, which consisted of the last time point and its lagged values (i.e., the right gray box), for prediction. In contrast, we use the information of the nearest neighbors of **all** of the windows.

We use the Matrix Profile [15, 16] to annotate the nearest neighbor for each m -subsequence of a time series T of length n . The distance is the z-normalized Euclidean distance. It may seem computationally expensive to perform this annotation at first glance. Algorithm 1 shows the brute force approach to compute the matrix profile. The two for-loops and the computation of z-normalized Euclidean distance, which takes $\mathcal{O}(m)$, indicate that the computational complexity is $\mathcal{O}(n^2m)$. The space complexity is $\mathcal{O}(n^2)$ because of the pairwise distance of each subsequence with the other subsequence. However, the matrix profile can be computed in $\mathcal{O}(n^2)$ using an exact method, namely STOMP [15] or its community-open-sourced version, STUMP [17]. Besides, the running time can be further sped up by parallelization for a single machine with multiple computation units, such as CPUs or GPUs. The tool also allows us to compute the left matrix profile to find the left nearest neighbor of each window. To note, the matrix profile annotates a time series with information about the nearest neighbor of each subsequence, including the similarity with its nearest neighbor and its location, as shown in Figure 1.2.

In this study, we make the following contributions:

- We are the first to propose leveraging the matrix profile to create meaningful covariates that improve forecaster performance.

- We have proposed two methods namely, GBRT-NN, which uses the immediate subsequence as the covariates, and GBRT-NN-S, which also involves the similarity on top of GBRT-NN, as the covariates. 95
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- Experimental results show that our approach can improve the GBRT forecaster in most cases, with a very small cost to compute the matrix profile. 98
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The rest of this study is organized as follows. Section 1.2 presents the related-work. In Section 1.3, we introduce the necessary background knowledge, then introduce our method. Section 1.4 contains an empirical evaluation. Finally, we conclude this study and provide future work in Section 1.5. 100
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1.2 Related Work

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Many methods have been developed for time series forecasting. Traditional methods include rolling averages (RA), vector auto-regression (VAR) [1, 18], and auto-regressive integrated moving averages (ARIMA) [19, 20, 18]. Because of their rigorous statistical properties, they have long been the standard. The shortcomings of ARIMA and its variants include their high computational cost [1]. In contrast, VAR is arguably the most widely used method, particularly in multivariate time series analysis, owing to its simplicity. However, most of these traditional approaches have certain limitations. They perform well when the data meet specific statistical assumptions, such as stationarity [21], which means that the mean and variance of the time series remain constant over time. It motivates the community to develop machine learning methods, particularly deep learning methods for time series forecasting. Many deep learning models have been proposed, including RNN-based models, CNN-based models, GNN-based models, Transformer-based models, and compound models that incorporate different base models mentioned before [6]. The compound models are promising. For example, RNNs are well suited to capturing long-term dependencies, whereas CNNs are well suited to capturing short-term dependencies. A good way to improve performance is to compound them. For example, LSTnet [1] integrates CNN, RNN, and autoregressive [22] techniques to extract both short-term and long-term patterns. Using the occupancy rate of a freeway as an example [1] to explain these two patterns, the “short-term” patterns refer to the morning peaks against evening peaks, while the “long-term” patterns refer to the workday patterns against weekend patterns. Clearly, a good forecaster needs to capture and distinguish both kinds of patterns. Despite the superior performance deep learning methods have achieved, they tend 105
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129 to be overly complex, opaque, and incur high computational costs compared to
130 traditional techniques.

131 1.3 Method

132 In this section, we first formulate the time series forecasting problem, followed
133 by the evaluation method. We then explain how to use a Gradient Boosting Re-
134 gression Tree (GBRT) for forecasting. Subsequently, we discuss how to leverage
135 the nearest neighbors' information of each subsequence to improve GBRT's per-
136 formance. Finally, we discuss how to compute those nearest neighbors using the
137 Matrix Profile.

138 To begin, we define the data type of interest: time series.

139 **Definition 1** (Time series). A *time series* $T = t_1, t_2, \dots, t_n$ is a sequence of real-
140 valued numbers with length $= n$.

141 In Definition 1, T is a univariate time series where each entry is a scalar
142 number. If each entry is a vector consisting of scalar numbers with size > 1 , T is a
143 multivariate time series. A multivariate time series can be regarded as a sequence
144 of vectors. It can also be represented as a vector of univariate time series, where
145 each univariate time series is referred to as a channel. In a dataset with more than
146 one time series, we use T_i to denote a time series in a dataset with N time series,
147 where $1 \leq i \leq N$.

148 The local properties of T can be analyzed through its subsequences.

149 **Definition 2** (Subsequence). A *subsequence* $T_{i,m} = t_i, t_{i+1}, \dots, t_{i+m-1} = t_{i:i+m-1}$
150 of a T is a sequence that consists of a continuous subset of the entries from T of
151 length m starting from i .

152 1.3.1 Problem Formulation

153 Time series forecasting is the task of predicting h -future values $y_{t+1}, y_{t+2}, \dots, y_{t+h}$
154 of a target Y at the current time point t . In this study, there is only one target
155 variable Y . h is the number of steps we want to predict in the future. The simplest
156 case is one-step-ahead forecasting, where $h = 1$. The predicted value is denoted
157 as \hat{y}_{t+1} where the actual value is y_{t+1} . It is preferable to predict multiple points in
158 the future. It is called multi-horizon (multi-step) forecasting, where $h > 1$. The
159 task of forecasting is encoded in Equation 1.1.

$$\hat{y}_{t+\tau} = f(y_{t-w+1:t}, x_{t-w+1:t}, u_{t-w+1:t+\tau}, \tau) \quad (1.1)$$

where

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- $\hat{y}_{t+\tau}$ is a prediction of the target value at $t + \tau$, where $\tau \in \{1, 2, \dots, h\}$.
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- $y_{t-w+1:t}$ are the actual values consisting of the current value y_t and the lag
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values before it. y_{t-i} is called the lag of i or i -lag.
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- x_t are inputs that can only be known historically at time t . x_{t+1} is not known
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at t .
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- u_t are known inputs for all time. For example, the date information such
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as the day of the week or month [21]. Even at t , u_{t+i} where $1 \leq i \leq \infty$ are
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known.
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x_t and u_t are called covariates of y_t . The input of Equation 1.1 is a look-back
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window w .
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We explain the task of forecasting in terms of Equation 1.1. The forecasting
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process estimates the value of $y_{t+\tau}$, denoted by $\hat{y}_{t+\tau}$ with the aim to minimize
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the error function, typically represented as a function of $y_{t+\tau} - \hat{y}_{t+\tau}$ for each τ .
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It is obvious that date information is useful when the target variable depends
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on when the measurement is taken. For example, if the target variable is the
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electricity consumption rate, there is a clear pattern by month: consumption is
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higher during the winter and summer months, when air conditioners and heaters
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are used. x_t provides additional information about the state of y_t . For example,
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if the target variable is the body temperature, and x_t tells us the severity of the
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sore throat, we may guess the body temperature will raise tomorrow.
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1.3.2 Evaluation Method

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Given a dataset D of N time series T_i , where $1 \leq i \leq N$, we explain how to
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evaluate the performance of a forecaster on T_i . The error made by the forecaster
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on D is simply the summation of errors made by the forecaster on each T_i . We
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now focus on a single time series; hence, we drop the index i . T is divided into
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two subsequences, namely training subsequence T_{train} and test subsequence T_{test} .
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In our study, the forecaster is only allowed to train on T_{train} . Recall that we
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are predicting the h future values from the w values just before them. Hence, we
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use a sliding window of length $w + h$ to generate the w -predictor- h -response pairs
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in T_{train} , enabling the forecaster to train on them. During the test (evaluation)
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phase, we do rolling forecasts. We predict based on the ground truth, not results
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generated from the model. It is used to prevent the accumulation of errors.
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193 This concept is called “Teacher forcing” [23] because the teacher’s values are
 194 “force fed” into the forecaster when we “roll” the forecaster on the T_{test} [24]. The
 195 intuition is that, suppose each question (except the first one) in an exam depends
 196 on the answers to the previous questions, rather than simply grading every answer
 197 in the end, a teacher would grade (evaluate) the answer once it is given by the
 198 student, and provide the correct answer to the student so he can answer the next
 199 question based on the correct answer.

200 To evaluate the forecaster, we used the following three evaluation metrics de-
 201 fined as:

- 202 • Root Mean Square Error (RMSE)

$$\text{RMSE} = \sqrt{\frac{1}{n} \sum_{i=1}^n (y_i - \hat{y}_i)^2} \quad (1.2)$$

- 203 • Weighted Absolute Percentage Error (WAPE)

$$\text{WAPE} = \frac{\sum_{i=1}^n |y_i - \hat{y}_i|}{\sum_{i=1}^n |y_i|} \quad (1.3)$$

- 204 • Mean Absolute Error (MAE)

$$\text{MAE} = \frac{1}{n} \sum_{i=1}^n |y_i - \hat{y}_i| \quad (1.4)$$

205 where n is the length of the time series, y_i , \hat{y}_i is ground true value and predicted
 206 value, respectively. RMSE and MAE are widely used metrics. MAE can better
 207 reflect the actual error situation than RMSE [4]. WAPE was introduced by [25].
 208 By rewriting Equation 1.3 to Equation 1.5, it is more obvious that it is a weighted
 209 absolute percentage error.

$$\text{WAPE} = \sum_{i=1}^n w_i \frac{|y_i - \hat{y}_i|}{|y_i|} \quad (1.5)$$

210 where the weights are given by

$$w_i = \frac{|y_i|}{\sum_{i=1}^n |y_i|} \quad (1.6)$$

211 For all of them, a lower value is better.

1.3.3 Gradient Boosting Regression Tree (GBRT)

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Gradient boosting [26] is a boosting algorithm that ensembles a group of weak
213 learners (usually decision trees) to make predictions. It sequentially adds learners
214 to an ensemble, with each learner connecting its predecessor. It constructs weak
215 learners in a way that each learner strategically corrects the predecessor’s mistakes
216 by fitting the new learner to the residual errors made by the predecessor [27, 28].
217 It can be used in classification and regression. In this study, we focus on its use
218 in regression. For the usage in regression, the model is called “Gradient Boosting
219 Regression Tree (GBRT)”. Some popular optimized implementations of gradient
220 boosting are XGBoost [29], CatBoost [30], and LightGBM [31]. In this study, we
221 use XGBoost.
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In order to apply GBRT into time series forecasting problem, we need to cast
223 the input into an appropriate format to input into GBRT. The casting approach
224 is similar to successful time-series forecasting models, which reconfigure the time
225 series into windowed inputs [19]. Figure 1.1 presents the reconfiguration. For
226 each entry of the target variable y_i , we retrieve its u_i , such as the day information
227 from the calendar. Hence, for each y_i , it is associated with x_i and u_i . To simplify
228 the notation, we absorb u_i into x_i , and it is called the covariates of y_i . The 2D
229 window, as shown on the left-hand side in Figure 1.1, with size $w \times M$, where M
230 is the total number of covariates, is flattened into a 1D array on the right-hand
231 side with length $w + M$. To note, as suggested in the literature [19], only the
232 covariates of the last time-point i are kept and appended to the final vector. By
233 reconfiguration, we obtain the predictor-response pairs for training. In detail, the
234 predictor is $\textcolor{red}{y_{i-w+1}, y_{i-w+2}, \dots, y_i}$, $\textcolor{blue}{x_i^1, x_i^2, \dots, x_i^M}$ where the red part refers to the
235 current target value $\textcolor{red}{y_i}$ and its lag values, and the blue part refers to the covari-
236 ates of $\textcolor{red}{y_i}$. The corresponding output is $y_{i+1}, y_{i+2}, \dots, y_{i+h}$, with length = h . We
237 predict the h -horizon from the w -look back window (i.e., $w + M$ -flattened predic-
238 tor). With this predictor-response formulation, the forecasting problem becomes a
239 multi-output regression problem. Standard XGBoost cannot return a sequence of
240 predicted values; it only returns a single number [19]. To note, a multi-output re-
241 gression problem is simply a group of single-output regression problems. In other
242 words, XGBoost internally simply treats the prediction of h -steps as h individual
243 problems. Hence, the final output is produced by the h regressors rather than
244 by a single model. One may argue that the h regressors operate individually and
245 hence the temporal relationship in the output sequence is lost. However, as the
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247 individual regressors are trained on the same flattened input, the prediction would
248 still preserve the temporal relationship [19].

249 1.3.4 Matrix Profile

250 Our proposed method has a simple intuition. We would like to create covariates for
251 each time point in the time series, as in the case of using the date information to
252 create the covariates. For example, given the timepoint date (2026-02-01, 14:38),
253 we can deduce the minute (38), hour (14), day (1), month (2), and year (2026).
254 Besides, by reading the calendar, the day of the week (Sunday), the day of the year
255 ($31+1=32$), the week of the year (the firth week in 2026) can also be obtained.
256 Given a time point t_p in T , and a user-given m , we want to use the m -subsequence
257 with t_p as the ending point as a query Q , and to find its left m -subsequence that
258 is the nearest neighbor of Q . Hence, the immediate subsequence of the nearest
259 neighbor informs us of the dynamics of the immediate subsequence of Q . In
260 Figure 1.2, the red triangle in the right gray box is t_p and the right gray box is
261 Q . We seek its leftmost nearest neighbor, which turns out to be the left gray box.
262 Note that we would like to perform this operation for each point t_p in the time
263 series T , $m \leq t_p \leq |T|$.

264 We discuss how to use a data primitive called Matrix Profile [15, 16] for this
265 operation. In brief, a matrix profile P is a time series that annotates an input time
266 series T , storing the z-normalized Euclidean distance between each m -subsequence
267 and its nearest neighbor in T . Besides, another supplementary time series, namely
268 the Matrix Profile Index I , stores the location of the corresponding nearest neigh-
269 bor. To begin with, we first define the distance profile of T .

270 **Definition 3** (Distance profile). A *distance profile* $D_i = d_{i,1}, d_{i,2}, \dots, d_{i,n-m+1}$
271 of a T is a vector of the Euclidean distances between a given subsequence $T_{i,m}$
272 and each subsequences in T , where $d_{i,j}$ is the distance between $T_{i,m}$ and $T_{j,m}$,
273 $1 \leq i, j \leq n - m + 1$.

274 The distances are measured between z-normalized time series. Equipped with
275 the distance profile, we know all the Euclidean distances between a given subse-
276 quence $T_{i,m}$ and each subsequences in T . From this, we define the matrix profile
277 P and its supplementary matrix profile index I as follows.

278 **Definition 4** (Matrix profile). A *matrix profile* $P = \min(D_1), \min(D_2), \dots,$
279 $\min(D_{n-m+1})$ of T is a vector of Euclidean distances between every subsequence
280 $T_{i,m}$ of T and its nearest neighbor in T .

Definition 5 (Matrix profile index). A *matrix profile index* $I = I_1, I_2, \dots, I_{n-m+1}$ of T is a vector of integers, where $I_i = j$ if $d_{i,j} = \min D_i$. 281
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In this study, instead of the general matrix profile (index), we are interested in the left version of it. The left version of the matrix profile informs us of the information about the left nearest neighbor of any m -subsequences in T . It is shown in Figure 1.2. The left matrix profile has high values in the beginning because they can only find the left neighbor, and there are few left subsequences. In contrast, right matrix profile has low values in the beginning because there are many right subsequences To note, each entry i in Matrix Profile P_i is simply the min of P_i^L and P_i^R (i.e., $P_i = \min(P_i^L, P_i^R)$). 283
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Definition 6 (Left distance profile). A *left distance profile* $D_i^L = d_{i,1}, d_{i,2}, \dots, d_{i,i-\lceil m/4 \rceil - 1}$ of T is a vector of Euclidean distances between a given subsequence $T_{i,m}$ and each subsequence that appears before $T_{i,m}$. To note, $i - \lceil m/4 \rceil - 1$ is the index location of the last eligible subsequence before $T_{i,m}$ because of the exclusion zone. 291
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We discuss the idea of an exclusion zone. For a given m -subsequence Q , the distance profile is zero at the location of Q (because Q must be a nearest neighbor of Q) and close to zero just before and after it. But the corresponding m -subsequences are trivial matches of Q . We need to define a zone, namely an exclusion zone, for this region. It is defined as $m/2$ before and after the location of Q [15]. The community implementation uses $m/4$ instead [17]. 296
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Definition 7 (Left matrix profile). A *left matrix profile* $P^L = \min(D_1^L), \min(D_2^L), \dots, \min(D_{n-m+1}^L)$ of T is a vector of Euclidean distances between every subsequence $T_{i,m}$ of T and its nearest neighbor in T before it. 302
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Definition 8 (Left matrix profile index). A *left matrix profile index* I^L is a vector of integers $I_1^L, I_2^L, \dots, I_{n-m+1}^L$ of T , where $I_i^L = j$ if $d_{i,j} = \min D_i^L$. 305
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Note that the original indexing system in Matrix Profile uses the start point rather than the end point to define the subsequence. In Figure 1.2, the matrix profile is shown in the original definition. The gray boxes are associated with the start point. Hence, the red Matrix Profile starts at $t = 1$ rather than $t = m$. To facilitate our discussion, from now on, we refer to Matrix Profile and its variants using the index defined on the end point instead of the start point. Formally, we use the entries of Matrix Profile at $i - m + 1$ to be the matrix profile at i in our indexing system. Visually speaking, we shift the matrix profile to the right by $m - 1$. 307
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316 To conclude this part, given the left matrix profile (index), we can compute, for
 317 each m -subsequence in T , the information on its left nearest neighbor, including its
 318 similarity and location. Besides, with the location (it now refers to the end point
 319 of the subsequence), we can retrieve the points after it and form the immediate
 320 subsequence with length = h of the nearest neighbor.

321 A natural setting for m and the size of the immediate subsequence would be
 322 the w and h as defined in Figure 1.1, respectively.

323 1.4 Experiments

Table 1.1: Dataset Statistics. N is the number of time series in the dataset, while $|T| = n$ is the length of each time series. “rate” refers to the measuring rate. w is the size of the look-back window. h is the size of the forecasting window, also known as the forecasting horizon. T_{train} is the training subsequence of T . T_{test} is the test subsequence of T . To note, $|T_{\text{train}}| + |T_{\text{test}}| = n$.

Dataset	Data			Forecasting Task		
	N	n	rate	w, h	$ T_{\text{train}} $	$ T_{\text{test}} $
Electricity [32]	70	26,136	hourly	24	25,968	168
Traffic [32]	90	10,560	hourly	24	10,392	168
PeMSD7 [32]	228	12,672	/5 mins	9	11,232	1,440
Exchange-Rate [1]	8	7,536	daily	24	6,048	1,488

324 The code and data are available at <https://github.com/colemanyu/matri>
 325 **x-profile-motif-forecasting**. In this study, we focus on univariate time series
 326 forecasting. There is only one single target variable Y . We predict the future of
 327 Y only based on the past of it. The dataset used is listed in Table 1.1. For each
 328 time series T in the dataset, it is split into two contiguous time series, namely
 329 $T_{\text{train}} = T(1 : \text{split})$ and $T_{\text{test}} = T(\text{split} + 1 : |T|)$, where split defines the training-
 330 test split, which is shown in the column 6 in Table 1.1. To note, the N time
 331 series in a dataset are considered as multiple, independent univariate time series
 332 instead of a multivaraite time series with channels = N . The original covariates
 333 are constructed from the timestamp information. The settings of w and h are
 334 adopted from the original corresponding papers [19]. It is not necessary for them
 335 to be the same.

336 GBRT-NN refers to a model that incorporates immediate sequence informa-
 337 tion. GBRT-NN-S refers to a model that incorporates immediate sequence infor-

mation with the similarity information. The experimental results are shown in 338
Table 1.2 and Table 1.3. 339

Table 1.2: Experimental Results without original covariates (bold represents the best result and underlined represents the second best) (* refers to the results reported from [19]) (For the GBRT-related methods, we round to the nearest 4 decimal places for better comparison, for the others, we round to the 3 decimal places).

Dataset	Metric	LSTNet* [1]	TRMF* [33]	DARNN* [34]	ARIMA* [35]	GBRT [19]	GBRT-NN	GBRT-NN-S
Electricity [32]	RMSE	1095.309	<u>136.400</u>	404.056	181.210	136.254	142.035	138.354
	WAPE	0.997	0.095	0.343	0.310	0.103	0.101	<u>0.100</u>
	MAE	474.845	53.250	194.449	154.390	57.929	56.464	<u>55.972</u>
Traffic [32]	RMSE	0.042	0.023	0.015	0.044	<u>0.012</u>	0.016	0.008
	WAPE	0.102	0.161	0.132	0.594	0.108	<u>0.079</u>	0.037
	MAE	0.014	0.009	0.007	0.032	0.006	<u>0.004</u>	0.002
PeMSD7 [32]	RMSE	55.405	5.462	5.983	15.357	5.610	5.575	<u>5.557</u>
	WAPE	0.981	<u>0.057</u>	0.060	0.183	0.051	0.051	0.051
	MAE	53.336	3.329	3.526	10.304	2.984	<u>2.965</u>	2.957
Exchange-Rate [1]	RMSE	0.018	0.018	0.025	0.123	0.020	<u>0.019</u>	<u>0.019</u>
	WAPE	0.017	0.015	0.022	0.170	<u>0.016</u>	0.015	0.015
	MAE	0.013	0.011	0.016	0.101	<u>0.012</u>	<u>0.011</u>	<u>0.012</u>

Table 1.3: Experimental Results with original covariates (bold represents the best result and underlined represents the second best) (* refers to the results reported from [19]).

Dataset	Metric	DeepGlo* [32]	GBRT [19]	GBRT-NN	GBRT-NN-S
Electricity [32]	RMSE	141.285	132.669	123.591	<u>124.215</u>
	WAPE	0.094	0.0929	0.089	0.089
	MAE	53.036	52.0232	49.606	<u>49.739</u>
Traffic [32]	RMSE	0.026	<u>0.014</u>	0.018	0.009
	WAPE	0.239	0.109	<u>0.101</u>	0.062
	MAE	0.013	0.006	<u>0.006</u>	0.003
PeMSD7 [32]	RMSE	6.490	5.191	<u>5.163</u>	5.156
	WAPE	<u>0.070</u>	0.048	0.048	0.048
	MAE	3.530	2.796	<u>2.779</u>	2.778
Exchange-Rate [1]	RMSE	0.038	<u>0.020</u>	0.019	0.019
	WAPE	0.038	<u>0.016</u>	0.015	0.015
	MAE	0.029	0.012	0.012	0.012

1.5 Concluding Remarks

340

1.5.1 Future Work

341

Leveraging nearest neighbors' location information: It would be beneficial 342
to retrieve the nearest neighbors for each subsequence in a specific range with 343
respect to it. Real-world applications often require the separation of information 344

345 of short-term and long-term repeating patterns for making accurate predictions [1].
346 Notably, the matrix profile also provides the locations of the nearest neighbors from
347 the matrix profile index. Using this location (index) information, we can retrieve
348 the nearest neighbors of each subsequence in a specified range with respect to it
349 to find those “short-term” and “long-term” patterns.

350 **Extend to multidimensional case:** This study focuses on univariate time series
351 forecasting, where there is a single target and no exogenous inputs. It only requires
352 us to find one-dimensional nearest neighbors. When there are multiple targets or a
353 single target with multiple exogenous inputs, we need to identify multidimensional
354 nearest neighbors [36] and leverage their information for forecasting.

355 **Top- k neighbors and motifs:** A simple extension is to consider the information
356 not just from the nearest neighbor but from the k -nearest neighbors. Besides, we
357 can use motifs instead of neighbors to obtain more stable “future” information for
358 each window. Recall that a time series motif is a repeated pattern that consists
359 of at least two occurrences. A motif can be considered as a family of nearest
360 neighbors A nearest neighbor is a historical occurrence that instantiates this motif.
361 The motif captures the ideal behavior. By finding the occurrences of a motif and
362 considering their immediate subsequences, we can make a more confident guess
363 about this motif. We outline the approach for finding members of a motif¹ Given
364 a subsequence A in a time series T , we denote the left-hand side of A in T as T_L .
365 We find A ’s nearest neighbor in T_L , denoted as B . They are the two members of
366 a motif M . We want to identify other subsequences in T_L that belong to M . We
367 define a threshold $\theta = r \times \text{ED}(A, B)$, where $r > 1$. The center M_C of M is defined
368 as the average of A and B . Then, we compute the distance profile between M_C
369 and T_L . Any part of the distance profile that is smaller than θ points to a member
370 of M in T_L . These members can then be added to M . After identifying all the
371 members of M and excluding these members in the next consideration, we can find
372 the next left nearest neighbor of A in T_L , and repeat the same process for finding
373 the next motif. Given a set of immediate subsequences of members (occurrences)
374 of M , we can compute a more stable immediate subsequence (future) associated
375 with M by excluding the outliers among them or using the ensemble value, such
376 as the mean or median of them, to cancel the noise.

377 **Identify outliers of immediate subsequences:** When we have a set of im-
378 mediate subsequences, we can determine whether an immediate subsequence is an
379 outlier or not by comparing it with others. We provide a heuristic to identify an
380 outlier as follows. Recall that the length of a nearest neighbor and its immediate

¹The idea has been mentioned in <https://www.cs.ucr.edu/~eamonn/TimeSeriesMotifs/>.

subsequence is m and h , respectively. We concatenate all nearest neighbors into a single long time series T' . To establish a clear boundary, we append a NaN value after each of them. It ensures that all matrix profile computations do not consider subsequences that span multiple neighbors. Then, we compute a distance profile of T' to find the nearest neighbor distance d_i of each neighbor i . Let S_i be the sequence consisting of neighbor i of length m and its immediate subsequence of length h . The expected nearest neighbor distance of S_i (found within the set of all extended sequences) should be proportional to the increase in length: $d_i \times \frac{m+h}{m}$. If the actual nearest neighbor distance of S_i is greater than $r' \times (d_i \times (m+h)/m)$ among the others, where r' is a user-given value, the immediate subsequence in S_i is considered as an outlier.

Bibliography

392

- [1] G. Lai, W.-C. Chang, Y. Yang, and H. Liu, “Modeling long- and short-term temporal patterns with deep neural networks,” in *The 41st International ACM SIGIR Conference on Research & Development in Information Retrieval*, ser. SIGIR ’18. New York, NY, USA: Association for Computing Machinery, Jun. 2018, pp. 95–104. 393
394
395
396
397
- [2] C. Chatfield, *The Analysis of Time Series: An Introduction, Sixth Edition*, 6th ed. New York: Chapman and Hall/CRC, Jul. 2003. 398
399
- [3] O. Y. Al-Jarrah, P. D. Yoo, S. Muhaidat, G. K. Karagiannidis, and K. Taha, “Efficient machine learning for big data: A review,” *Big Data Research*, vol. 2, no. 3, pp. 87–93, Sep. 2015. 400
401
402
- [4] W. Li and K. L. E. Law, “Deep learning models for time series forecasting: A review,” *IEEE Access*, vol. 12, pp. 92 306–92 327, 2024. 403
404
- [5] N. I. Sapankevych and R. Sankar, “Time series prediction using support vector machines: A survey,” *IEEE Computational Intelligence Magazine*, vol. 4, no. 2, pp. 24–38, May 2009. 405
406
407
- [6] Z. Chen, M. Ma, T. Li, H. Wang, and C. Li, “Long sequence time-series forecasting with deep learning: A survey,” *Information Fusion*, vol. 97, p. 101819, Sep. 2023. 408
409
410
- [7] J. F. Torres, D. Hadjout, A. Sebaa, F. Martínez-Álvarez, and A. Troncoso, “Deep learning for time series forecasting: A survey,” *Big Data*, vol. 9, no. 1, pp. 3–21, Feb. 2021. 411
412
413
- [8] D. B. da Silva, D. Schmidt, C. A. da Costa, R. da Rosa Righi, and B. Eskofier, “Deepsigns: A predictive model based on deep learning for the early detection of patient health deterioration,” *Expert Systems with Applications*, vol. 165, p. 113905, Mar. 2021. 414
415
416
417

- 418 [9] N. Wu, B. Green, X. Ben, and S. O'Banion, “Deep transformer models for
419 time series forecasting: The influenza prevalence case,” Jan. 2020.
- 420 [10] F. Martínez-Álvarez, G. Asencio-Cortés, J. F. Torres, D. Gutiérrez-Avilés,
421 L. Melgar-García, R. Pérez-Chacón, C. Rubio-Escudero, J. C. Riquelme, and
422 A. Troncoso, “Coronavirus optimization algorithm: A bioinspired metaheuristic
423 based on the **COVID-19** propagation model,” *Big Data*, vol. 8, no. 4, pp.
424 308–322, Aug. 2020.
- 425 [11] M. Middlehurst, P. Schäfer, and A. Bagnall, “Bake off redux: A review and
426 experimental evaluation of recent time series classification algorithms,” *Data
427 Mining and Knowledge Discovery*, vol. 38, no. 4, pp. 1958–2031, Jul. 2024.
- 428 [12] F. Martínez, M. P. Frías, M. D. Pérez, and A. J. Rivera, “A methodology for
429 applying k-nearest neighbor to time series forecasting,” *Artificial Intelligence
430 Review*, vol. 52, no. 3, pp. 2019–2037, Oct. 2019.
- 431 [13] S. Tajmouati, B. E. L. Wahbi, A. Bedoui, A. Abarda, and M. Dakkon, “Ap-
432 plying k-nearest neighbors to time series forecasting: Two new approaches,”
433 *Journal of Forecasting*, vol. 43, no. 5, pp. 1559–1574, 2024.
- 434 [14] D. T. Thi, N. T. Phong, and N. D. Bui, “Forecast timeseries based on matrix
435 profile,” *Journal of Informatics and Innovative Technologies (JIIT)*, 2021.
- 436 [15] C.-C. M. Yeh, Y. Zhu, L. Ulanova, N. Begum, Y. Ding, H. A. Dau, D. F. Silva,
437 A. Mueen, and E. Keogh, “Matrix profile i: All pairs similarity joins for time
438 series: A unifying view that includes motifs, discords and shapelets,” in *2016
439 IEEE 16th International Conference on Data Mining (ICDM)*. Barcelona,
440 Spain: IEEE, Dec. 2016, pp. 1317–1322.
- 441 [16] Y. Zhu, M. Imamura, D. Nikovski, and E. Keogh, “Matrix profile vii: Time
442 series chains: A new primitive for time series data mining,” in *2017 IEEE
443 International Conference on Data Mining (ICDM)*, Nov. 2017, pp. 695–704.
- 444 [17] S. M. Law, “**STUMPY**: A powerful and scalable python library for time
445 series data mining,” *Journal of Open Source Software*, vol. 4, no. 39, p. 1504,
446 Jul. 2019.
- 447 [18] G. E. P. Box, G. M. Jenkins, G. C. Reinsel, and G. M. Ljung, *Time Series
448 Analysis: Forecasting and Control*. John Wiley & Sons, May 2015.

- [19] S. Elsayed, D. Thyssens, A. Rashed, H. S. Jomaa, and L. Schmidt-Thieme, “Do we really need deep learning models for time series forecasting?” Oct. 2021. 449
450
451
- [20] G. E. P. Box and D. A. Pierce, “Distribution of residual autocorrelations in autoregressive-integrated moving average time series models,” *Journal of the American Statistical Association*, vol. 65, no. 332, pp. 1509–1526, 1970. 452
453
454
- [21] B. Lim and S. Zohren, “Time-series forecasting with deep learning: A survey,” *Philosophical Transactions of the Royal Society A: Mathematical, Physical and Engineering Sciences*, vol. 379, no. 2194, p. 20200209, Feb. 2021. 455
456
457
- [22] G. U. Yule, “On a method of investigating periodicities in disturbed series, with special reference to Wolfer’s sunspot numbers,” *Philosophical Transactions of the Royal Society of London. Series A, Containing Papers of a Mathematical or Physical Character*, vol. 226, pp. 267–298, 1927. 458
459
460
461
- [23] R. J. Williams and D. Zipser, “A learning algorithm for continually running fully recurrent neural networks,” *Neural Computation*, vol. 1, no. 2, pp. 270–280, Jun. 1989. 462
463
464
- [24] K. P. Murphy, *Probabilistic Machine Learning: An Introduction*, ser. Adaptive Computation and Machine Learning. Cambridge, Massachusetts London, England: The MIT Press, 2022. 465
466
467
- [25] S. Kolassa and W. Schütz, “Advantages of the **MAD**/mean ratio over the **MAPE**,” *Foresight: The International Journal of Applied Forecasting*, vol. 6, pp. 40–43, 2007. 468
469
470
- [26] J. H. Friedman, “Greedy function approximation: A gradient boosting machine.” *The Annals of Statistics*, vol. 29, no. 5, pp. 1189–1232, Oct. 2001. 471
472
- [27] L. G. Serrano and S. Thrun, *Grokking Machine Learning*. Shelter Island: Manning, 2021. 473
474
- [28] A. Géron, *Hands-On Machine Learning with Scikit-Learn and PyTorch: Concepts, Tools, and Techniques to Build Intelligent Systems*. US: O’Reilly Media, 2025. 475
476
477
- [29] T. Chen and C. Guestrin, “**XGBoost**: A scalable tree boosting system,” in *Proceedings of the 22nd ACM SIGKDD International Conference on Knowl-* 478
479

- edge Discovery and Data Mining, ser. KDD '16. New York, NY, USA: Association for Computing Machinery, Aug. 2016, pp. 785–794.
- [30] A. V. Dorogush, V. Ershov, and A. Gulin, “**CatBoost**: Gradient boosting with categorical features support,” in *Workshop on ML Systems at NIPS 2017*, 2017.
- [31] G. Ke, Q. Meng, T. Finley, T. Wang, W. Chen, W. Ma, Q. Ye, and T.-Y. Liu, “**LightGBM**: A highly efficient gradient boosting decision tree,” in *Advances in Neural Information Processing Systems*, vol. 30. Curran Associates, Inc., 2017.
- [32] R. Sen, H.-F. Yu, and I. S. Dhillon, “Think globally, act locally: A deep neural network approach to high-dimensional time series forecasting,” in *Advances in Neural Information Processing Systems*, vol. 32. Curran Associates, Inc., 2019.
- [33] H.-F. Yu, N. Rao, and I. S. Dhillon, “Temporal regularized matrix factorization for high-dimensional time series prediction,” in *Advances in Neural Information Processing Systems*, vol. 29. Curran Associates, Inc., 2016.
- [34] Y. Qin, D. Song, H. Cheng, W. Cheng, G. Jiang, and G. W. Cottrell, “A dual-stage attention-based recurrent neural network for time series prediction,” in *Proceedings of the 26th International Joint Conference on Artificial Intelligence*, ser. IJCAI'17. Melbourne, Australia: AAAI Press, Aug. 2017, pp. 2627–2633.
- [35] S. Makridakis and M. Hibon, “**ARMA** models and the **Box–Jenkins** methodology,” *Journal of Forecasting*, vol. 16, no. 3, pp. 147–163, 1997.
- [36] C.-C. M. Yeh, N. Kavantzas, and E. Keogh, “Matrix profile vi: Meaningful multidimensional motif discovery,” in *2017 IEEE International Conference on Data Mining (ICDM)*, Nov. 2017, pp. 565–574.