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#### ABSTRACT

Time-series data contains temporal order information that can guide representation learning for predictive end tasks (e.g., classification, regression). Recently, there are some attempts to leverage such order information to first pre-train time-series models by reconstructing time-series values of randomly masked time segments, followed by an end-task fine-tuning on the same dataset, demonstrating improved end-task performance. However, this learning paradigm decouples data reconstruction from the end task. We argue that the representations learnt in this way are not informed by the end task and may, therefore, be sub-optimal for the end-task performance. In fact, the importance of different timestamps can vary significantly in different end tasks. We believe that representations learnt by reconstructing important timestamps would be a better strategy for improving end-task performance. In this work, we propose TARNet<sup>1</sup>, Task-Aware Reconstruction Network, a new model using Transformers to learn task-aware data reconstruction that augments end-task performance. Specifically, we design a datadriven masking strategy that uses self-attention score distribution from end-task training to sample timestamps deemed important by the end task. Then, we mask out data at those timestamps and reconstruct them, thereby making the reconstruction task-aware. This reconstruction task is trained alternately with the end task at every epoch, sharing parameters in a single model, allowing the representation learnt through reconstruction to improve end-task performance. Extensive experiments on tens of classification and regression datasets show that TARNet significantly outperforms state-of-the-art baseline models across all evaluation metrics.

#### **CCS CONCEPTS**

• Mathematics of computing  $\rightarrow$  Time series analysis; • Computing methodologies  $\rightarrow$  Supervised learning by classification; Supervised learning by regression.

 $^1 \rm Code$  is publicly available at https://github.com/ranakroychowdhury/TARNet

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#### **KEYWORDS**

Time series; self-supervision; data reconstruction; self-attention

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#### **1 INTRODUCTION**

Time-series data has domain-specific structural properties encoded in the temporal ordering of events. These intrinsic properties can provide a rich source of supervision besides target labels, which the state-of-the-art time-series models [2, 38] often neglect. Recently, time-series Transformer [37] leveraged this unlabeled data to craft a reconstruction task that masks time-series values of randomly chosen time segments and reconstructs them. The pre-trained model is then fine-tuned on an end task, by reusing the *same* data samples along with their labels, leading to improved performance over exclusively doing supervised learning on the end task.

However, this data reconstruction task precedes fine-tuning as a decoupled step, which means the representation learnt during reconstruction is not informed about the end task. Hence, such learnt representation may not be fully leveraged to perform optimally on the end task.

Depending on the end task, different properties of the given data may be useful for different end tasks. For example, consider the following end tasks using the same data collected from sensors in a building: predict the level of energy consumption (high, medium, low) and the occupancy status (occupied or not) of a room based on outdoor temperature and humidity, and light intensity and  $CO_2$ readings from a room. Energy consumption prediction task may be highly correlated to times when temperature is high (air conditioning stays on) or light intensity is high (lights are switched ON) while occupancy status may correlate to timestamps when  $CO_2$ level is high. Hence, depending on the end task, certain timestamps in the data may be more important than others for that task.

Generic learnt representations typically result from decoupled data reconstruction and end tasks. To optimize the performance for an end task, we customize the learnt representation for the end task in TARNet. We test and validate the hypothesis that a representation learnt by reconstructing data from timestamps important to the end task will yield improved performance over reconstruction

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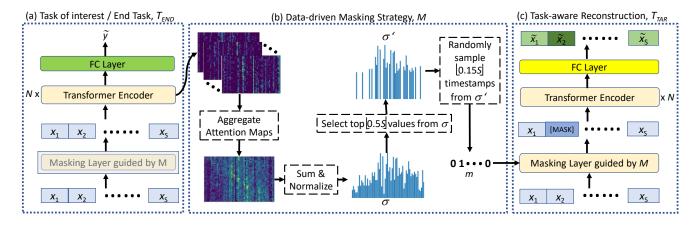


Figure 1: TARNet Overview: (a) Task of interest / End Task,  $T_{END}$ : Data is mean-standardized, then passed through an Embedding and a Positional Encoding layer (not shown for simplicity), followed by the N-layer Transformer Encoders and Fully Connected (FC) Layer; (b) Data-driven Masking Strategy, M: For every time-series data, we collect attention maps generated by Transformer Encoders in  $T_{END}$  and then compute the set of important timestamps to be masked in task-aware reconstruction; and (c) Task-aware Reconstruction,  $T_{TAR}$ : Input data are masked at timestamps computed by M and reconstructed. Transformer Encoder parameters are shared between  $T_{END}$  and  $T_{TAR}$ , but the FC layers are different (highlighted by different colors).

on random time segments. Therefore, we design a data reconstruction task which masks data from those important timestamps and reconstructs them. In the process, the model learns a task-specific representation, resulting in improved end task performance.

Figure 1 shows TARNet's learning process. Using a transformer encoder [29] as the backbone model, we train for the end task (Figure 1(a)) and the data reconstruction task (Figure 1(c)) alternately on the same model. In order to compute the timestamps to mask during data reconstruction, we design a data-driven masking strategy (Figure 1(b)). It uses the self-attention score distribution generated by transformer encoder during the end task training and determines the set of timestamps to mask. Since the two tasks share parameters, the representation learnt during reconstruction can be effectively leveraged by the end task to improve performance.

We conducted experiments on 34 classification datasets from UEA ARCHIVE [1], UCI MACHINE LEARNING REPOSITORY [10, 15] and 6 regression datasets from MONASH UNIVERSITY, UEA, UCR TIME SERIES REGRESSION ARCHIVE [27]. Time Series Transformer (TST) [37], the current state-of-the-art for time-series, achieved the best accuracy on 6 out of 10 datasets, when compared with 5 baselines. We compared TARNet with 14 state-of-the-art baselines and it performed the best on 17 out of 34 datasets, being 2.7% higher in average accuracy than TST, which now performs best on 7 datasets. Similarly, TST achieved the lowest error on 3 out of 6 datasets for regression when compared with 11 state-of-the-art baselines. TARNet achieved the lowest error on 3 and 2<sup>nd</sup> lowest error on 2 datasets when compared with the same baselines, whereas TST now achieves the lowest error on 2 and 2<sup>nd</sup> lowest error on 1 dataset. We conducted case studies to show how TARNet's data-driven masking strategy learns task-specific representations, consistent with domain characteristics, thereby boosting end-task performance.

In summary, our main contributions are:

• We propose TARNet to learn task-aware reconstruction from time-series data to augment end-task performance.

- We design a data-driven masking strategy to determine important timestamps to an end task and learn to reconstruct them.
- We evaluate TARNet on numerous real-world datasets to validate and quantify its efficacy compared with state-of-the-art methods.

#### 2 RELATED WORK

#### 2.1 Non-Deep Learning Methods

ROCKET [5] and MiniROCKET [6] recently produced state-of-the art results for time-series. They learn features extracted by numerous and various random convolutional kernels. Other relevant directions include: (1) time series shapelet, (2) bag-of-patterns, and (3) distance-based models. Baydogan et al. [3] introduced Symbolic Representation to learn local relationships between different dimensions. Shapelets [33] are short discriminative time series sub-sequences, e.g. dynamic shapelets [23], efficient shapelets [16]. WEASEL-MUSE [24] utilizes bag of SFA (Symbolic Fourier Approximation). Distance-based methods [8, 31] use distance metric to measure similarity of a pair of time series. Among limitations of these approaches are that they incorporate expert insights, consist of large, heterogeneous ensembles of classifiers, scale poorly to long time-series, and many apply to only uni-variate time-series.

TARNet can be applied to both uni- and multi-variate time-series, automatically extracts features, and handles long time-series.

#### 2.2 Deep Learning Methods

**Using labeled data.** Fawaz et al. [12] summarize many neural networks-based methods for time-series. Most neural networks-based methods use some arrangement of LSTM, CNN or both [18, 39]. Others use different components of neural models, e.g., learnable temporal pooling [19], correlative channel-aware learnable fusion [2], label-learning [22], attentional prototype network [38], and shapelet embedding [20]. TARNet proposes a subsidiary data reconstruction technique that utilizes knowledge from the end

task to learn a task-specific data representation. Sharing parameters of this reconstruction task with the end task in a single architecture allows the learnt representation to improve end task performance. **Using both unlabeled and labeled data.** Unsupervised representation learning for time-series uses triplet loss with negative sampling [14], hierarchical contrastive loss [36], temporal and contextual contrasting [11], local smoothness to define neighborhoods in time [28], and reprogramming acoustic models [32]. TST [37] first pre-trains a transformer model by an unsupervised objective; masks out time-series values at random time segments from data and reconstructs them. It then reuses the *same* training samples to fine-tune the model on an end task. This gave improved performance than using the data once to train a fully supervised model.

However, decoupling the data reconstruction from the end task makes the representation learnt during reconstruction uninformed about the end task. Depending on the end task, certain timestamps in time-series data may be more important than others [21], which the learnt representation ignores. TARNet aims to learn a taskaware data reconstruction by masking important timestamps with respect to the end task. Hence, the learnt representation is better suited for improving end task performance than the representation learnt from reconstructing randomly masked time segments.

#### **3 TARNET**

In Figure 1, we show a schematic diagram of TARNet common across all considered tasks. In this section, we first present the problem setting and base model architecture shared by the two tasks. Then, we explain the end-task  $T_{END}$  (i.e., Figure 1(a)) and task-aware reconstruction  $T_{TAR}$  (i.e., Figure 1(c)). Finally, we present our data-driven masking strategy (i.e., Figure 1(b)) that uses information from  $T_{END}$  to decide which timestamps to mask for  $T_{TAR}$ .

#### 3.1 Problem Description and Notations

Each training sample  $X \in \mathbb{R}^{S \times N}$  denotes a multivariate time-series of length *S* and *N* variables. Specifically, it comprises a sequence of *S N*-dimensional feature vectors,  $x_t \in \mathbb{R}^N : X \in \mathbb{R}^{S \times N}$ . This formulation also covers the uni-variate case when N = 1. All the training samples come together with a target label *y*, which is an integer class id for a classification task or a real-valued number for a regression task. The full training dataset is labeled, i.e. we do not leverage any additional unlabeled data. Based on these training samples, we build a model to predict the label  $\tilde{y}$  of unseen data X.

#### 3.2 Base Model

We opt to use Transformer Encoders [29] as the backbone model, as we aim to develop a general framework to learn task-specific reconstruction that can be applied for a multitude of tasks. An architecture consisting of an encoder provides flexibility as it can not only handle tasks like classification, regression, imputation, but also handle generative tasks such as forecasting. One can plug in a task of interest by replacing the Fully Connected (FC) Layer in Figure 1(a) by task-specific layers (e.g., decoder for forecasting).

The feature vectors  $x_t$  are first mean-standardized per variable dimension. Then  $x_t$  is linearly projected onto a *D*-dimensional vector space, where *D* is the dimension of the Transformer model sequence element representations (typically called embedding dimension):

$$u_t = \mathbf{W}_p x_t + b_p, \tag{1}$$

where  $W_p \in \mathbb{R}^{D \times N}$ ,  $b_p \in \mathbb{R}^D$  are learnable parameters and  $u_t \in \mathbb{R}^D$ , t = 1, 2, ..., S are the model input vectors. The Transformer is a feed-forward architecture insensitive to the ordering of input. Therefore, we add positional encoding to these input vectors in order to make it aware of the sequential nature of the time series. The resultant vectors become the queries, keys and values of the self-attention layer in the encoder block. We pass data through several layers of such Transformer encoder blocks. Then, we pass the output values weighted by self-attention scores through a fully connected feed-forward network. We refer the reader to the original work [29] for a detailed description of the Transformer model.

#### **3.3 End Task (** $T_{END}$ **)**

For clarity, we use classification and regression as example end tasks here. Please note that TARNet can be easily extended to other tasks such as anomaly detection and time-series forecasting, by tweaking the FC Layer in Figure 1(a).

We modify the base model architecture presented in Section 3.2 for regression and classification in the following way:

The data fed to  $T_{END}$  is not masked, as illustrated by the frozen Masking Layer in Figure 1(a). The vector corresponding to the last timestamp from Transformer Encoders  $z_t \in \mathbb{R}^D$  is fed through 2 FC layers and *RELU* activation (represented as f), with parameters

$$W_{L1} \in \mathbb{R}^{K_E \times D}, b_{L1} \in \mathbb{R}^{K_E}, W_{L2} \in \mathbb{R}^{K_E \times K_E}, b_{L2} \in \mathbb{R}^{K_E}$$

followed by the output layer with parameters

$$W_F^O \in \mathbb{R}^{C \times K_E}, b_F^O \in \mathbb{R}^C$$

where  $K_E$  is the feed-forward dimension of FC Layer for  $T_{END}$  and C is the number of classes for classification or number of scalars to be estimated for regression (typically C = 1):

$$\tilde{y} = W_E^O f(W_{L2} f(W_{L1} z_t + b_{L1}) + b_{L2}) + b_E^O.$$
(2)

For classification, predictions  $\tilde{y}$  are passed through a softmax to give probability distribution, p, over C classes. We use cross-entropy loss with categorical ground truth labels,  $\mathcal{L}_{END} = \sum_{i=1}^{C} y_i log(p_i)$ . For regression, we use squared error,  $\mathcal{L}_{END} = \|\tilde{y} - y\|_2^2$ .

#### **3.4** Task-aware Reconstruction (*T<sub>TAR</sub>*)

Learning data representation through reconstruction has been explored in natural language processing [7] and time-series [37]. The goal of  $T_{TAR}$ , illustrated in Figure 1(c), is to learn a data representation by reconstructing the input data X after it has been appropriately masked by the Data-driven Masking Strategy, M.

The role of TARNet's masking strategy M, elaborated in Section 3.5, is to generate a new binary training data mask  $m \in \mathbb{R}^S$  for each training sample at every epoch. It is a boolean array with  $\lfloor \mu S \rfloor$  number of 1's, where  $\mu$  is a hyper-parameter  $0 < \mu < 1$ , to select the timestamps to be masked from X for the reconstruction task. Let  $m_t$  represent the value of m at timestamp t. If  $m_t = 1$  we mask  $x_t$ , otherwise we do not. Masking a particular timestamp, t, involves replacing the *N*-dimensional feature vector  $x_t$  with zeros. X passes through Transformer Encoder layers after being masked

by *m*. The final representation vectors  $Z \in \mathbb{R}^{S \times D}$  is fed through 2 FC layers and *RELU* activation, with parameters

$$W_{L3} \in \mathbb{R}^{K_R \times D}, b_{L3} \in \mathbb{R}^{K_R}, W_{L4} \in \mathbb{R}^{K_R \times K_R}, b_{L4} \in \mathbb{R}^{K_R}$$

followed by the output layer with parameters

$$\mathbf{W}_{R}^{O} \in \mathbb{R}^{N \times K_{R}}, b_{R}^{O} \in \mathbb{R}^{N},$$

where  $K_R$  is the feed-forward dimension of FC Layer for  $T_{TAR}$  and N is the number of variables:

$$\tilde{X} = W_R^O f(W_{L4} f(W_{L3} Z + b_{L3}) + b_{L4}) + b_R^O.$$
(3)

The label for this task is the raw input data X. To ensure accurate reconstruction, we calculate Mean Square Error (MSE) between the ground truth X and prediction  $\tilde{X}$ . We calculate the average MSE loss for masked and unmasked part of the data as follows:

$$\mathcal{L}_{masked} = \frac{1}{N\sum_{t=1}^{S} m_t} \sum_{t=1}^{S} m_t \|\tilde{\mathbf{x}_t} - \mathbf{x}_t\|_2^2, \tag{4}$$

$$\mathcal{L}_{unmasked} = \frac{1}{N(S - \sum_{t=1}^{S} m_t)} \sum_{t=1}^{S} (1 - m_t) \|\tilde{x_t} - x_t\|_2^2.$$
(5)

Unlike TST, which only considers MSE loss for reconstructing the masked portion of the data,  $\mathcal{L}_{masked}$ , we include loss incurred for replicating the unmasked, observed portion of the input data,  $\mathcal{L}_{unmasked}$ , as well. Time-series data is auto-regressive with strong correlation across time. Therefore, the ability to reconstruct the masked data at a given timestamp depends on how effectively the model learns to reconstruct the unmasked data and use that as context to infer the masked data. Including the loss for the unmasked data ensures its accurate reconstruction.

The combined reconstruction loss  $\mathcal{L}_{TAR}$  is a weighted sum of  $\mathcal{L}_{masked}$  and  $\mathcal{L}_{unmasked}$ , given by

$$\mathcal{L}_{TAR} = \lambda \mathcal{L}_{masked} + (1 - \lambda) \mathcal{L}_{unmasked}, \tag{6}$$

where  $\lambda$  is a hyper-parameter  $0 < \lambda < 1$  that controls the relative weights between the two losses. It is advisable to keep  $\lambda > 0.5$  because the masked timestamps are more important for the end task than the unmasked ones.

With  $\mathcal{L}_{END}$  as the end task loss, the total loss becomes

$$\mathcal{L}_{Total} = \eta \mathcal{L}_{TAR} + (1 - \eta) \mathcal{L}_{END},\tag{7}$$

where  $\eta$  is a hyper-parameter ( $0 < \eta < 1$ ) that controls the relative weights between the two task losses. We train  $T_{END}$  and  $T_{TAR}$  end-to-end alternately at every epoch, until convergence.

#### **3.5 Data-driven Masking Strategy** (*M*)

Data reconstruction in Time-series Transformer [37] involves masking segment of time-series data at randomly chosen timestamps and reconstructing them. However, different timestamps in the data may have different levels of importance to the end task. Therefore, we eschew random reconstruction of data in favor of a strategy that uses end task characteristics. Specifically, we identify timestamps that the end task deemed *important* during learning. We will then mask  $x_t$  from X corresponding to those timestamps and reconstruct them during  $T_{TAR}$ . We hypothesize that reconstructing data at timestamps identified to be important by the end task will generate a data representation that benefits the end task. This is in contrast to a random masking based data reconstruction, which does not consider any such information.

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Algorithm 1 Training	of TARNet
Input: X, y	
<b>Hyper-parameters</b> : μ	, $\beta$ , $\lambda$ , $\eta$
Output: Model	
1: $\sigma$ initialized random	mly
2: Model = Transform	nerEncoder()
3: while training do	
4: $\sigma' = top \lfloor \beta S \rfloor va$	lues from $\sigma$
5: $m \sim \text{Randomly}$	sample $\lfloor \mu S \rfloor$ timestamps without replace-
ment from $\sigma'$	
6: $\tilde{X}, \tilde{y}, A = Model.$	$train(X, m) # A \leftarrow Self-Attention Scores$
7: Compute $\mathcal{L}_{TAR}$	$( ilde{X}, X, \lambda)$ and $\mathcal{L}_{END}( ilde{y}, y)$
8: $\mathcal{L}_{Total} = \eta \mathcal{L}_{TAI}$	$R + (1 - \eta) \mathcal{L}_{END}$
9: $\sigma = add\_and\_no$	rmalize(A)

10: end while

11: return Model

To define the notion of an "important" timestamp, we use selfattention weights generated by Transformer Encoder in the forward pass of  $T_{END}$ . Attention weights indicate how much weight should be assigned to each  $x_t$  to compute representation for a given  $x_t$ . We compute aggregate attention map  $A \in \mathbb{R}^{S \times S}$  by summing the attention maps generated by each layer of Transformer Encoder. Let  $A_{ik}$  be the attention weight assigned to  $x_k$  during update of  $x_i$ , where i = k = 1, 2, ..., S, and  $\sum_{k=1}^{S} A_{ik} = 1$  for all *i*. Therefore, the update to  $x_i$  is a weighted sum of  $x_{1,2,...,S}$ , where the weights are  $A_{i,k=1,2,...,S}$ . We compute  $\sigma \in \mathbb{R}^S$ , where  $\sigma_k = \frac{\sum_{k=1}^{S} A_{ik}}{\sum_{k=1}^{S} \sum_{i=1}^{S} A_{ik}}$ for k = 1, 2, ..., S.  $\sigma_k$  represents the normalized aggregate attention weight of timestamp k to the computation of  $x_1, x_2, ..., x_S$ . We define the importance of each timestamp by its magnitude in  $\sigma$ , i.e. the higher  $\sigma_k$  is, the more important timestamp k is for  $T_{END}$ .

We then select the timestamps corresponding to the top  $\lfloor \mu S \rfloor$  values in  $\sigma$  and mask them from X for reconstruction. Since the same training data is fed at every epoch, the set of important timestamps computed from a given sample will not vary across epochs. Hence, the model may memorize reconstructing a few selected timestamps from the sample, leading to *overfitting*. Considering the heterogeneity in time-series data due to irregular sampling frequency or uncertainty about feature availability, it is probable that real-world data may have a different set of important timestamps compared to those seen in training data. Therefore, not exploring enough timestamps to approximate the training data distribution may lead to poor generalization on the real-world data.

Hence, we ensure that for every sample, at each epoch the model explores a random set of timestamps among those that are important. Therefore, we introduce an attention regularization parameter,  $\beta$ , where  $\beta > \mu$  and  $0 < \beta < 1$ . We, therefore, compute set  $\sigma'$  to choose the top  $\lfloor \beta S \rfloor$  values in  $\sigma$ . Then we randomly sample  $\lfloor \mu S \rfloor$  timestamps without replacement from  $\sigma'$  to generate the training data mask m.  $m_t = 1$  if t is sampled from  $\sigma'$ , otherwise 0.

Although we still choose an important set of timestamps to mask, the use of randomization through sampling ensures that the model does not always mask the same set of timestamps for a sample throughout its entire training regime. This gives the model a more versatile representation of the underlying data distribution, yet, one that is important for the end task. This data-driven masking strategy makes the model learn task-specific data representation by reconstructing data at those timestamps deemed important by the end task. Algorithm 1 outlines the training procedure of TARNet.

### **4 EXPERIMENTS**

We present the datasets, baselines, training settings, followed by the evaluation metrics. We then show and analyze classification and regression results of TARNet. We also conduct an ablation study, few-shot training experiments and case studies to justify TARNet.

#### 4.1 Experimental Setup

We use benchmark time-series datasets with detailed information available in UEA ARCHIVE [1], UCI MACHINE LEARNING REPOSI-TORY [10, 15], and MONASH UNIVERSITY, UEA, UCR TIME SERIES REGRESSION ARCHIVE [27]. These datasets represent an assortment of domains (Motion, Audio, EEG, HAR), sensor type, and sampling frequency. The number of training data points varies from 15 to over one million, the length of the time series, *S*, varies between 8 to 17, 984, the number of features, *N*, varies between 1 to 1, 345, and the number of target classes, *C*, varies between 2 to 39. *N* = 1 covers the uni-variate case. *N* > 1 refers to the multi-variate case.

We compare TARNet with statistical [1, 4–6, 9, 24–26] and deep learning [11–14, 18, 20, 28, 30, 35, 37, 38] baselines.

- 4.1.1 Statistical Baselines.
- Distance-based method [1]. Euclidean Distance (ED), dimension independent dynamic time warping (DTWI), and dimensiondependent dynamic time warping (DTWD) [25].
- (2) SVR: [9] Support Vector Regression.
- (3) Tree-based methods: Random Forest [26] and XGBoost [4].
- (4) WEASEL-MUSE [24] is a bag-of-pattern based sliding-window approach with statistical feature extraction and filtration.
- (5) **Rocket** [5] convolves time series with random convolutional kernels and applies global max pooling to extract features.
- (6) MiniRocket [6] upgrades Rocket by speeding it up, using a small, fixed set of kernels, and is almost entirely deterministic.
- 4.1.2 Deep Learning Baselines.
- FCN [30] Fully Convolutional Networks. Replaces traditional final FC layer with a Global Average Pooling (GAP) layer.
- (2) MLSTM-FCNs [18] expands LSTM-FCN and Attention LSTM-FCN by adding squeeze-and-excitation blocks.
- (3) **Negative samples (NS)** [14] generates negative samples and trains a dilated causal convolution encoder with triplet loss.
- (4) **TapNet** [38] designs random group permutation method with multi-layer convolutional and attentional prototype network.
- (5) ShapeNet [20] extends shapelet [33] for multivariate timeseries. Learns shared embedding space across different shapelet candidates, trains a dilated causal CNN, followed by an SVM.
- (6) Time Series Transformer (TST) [37] pre-trains Transformer Encoder by masking random time segments and reconstructing them. Reuses the same data to fine-tune the model.
- (7) TS2Vec [35] performs hierarchical contrastive learning over augmented context views. Builds representation of an arbitrary sub-sequence by aggregating representations of timestamps.

- (8) TNC [28] leverages local smoothness of a signal to define temporal neighborhoods and learns generalizable representations.
- (9) **TS-TCC** [11] encourages consistency of different data augmentations to learn transformation-invariant representations.
- (10) ResNet [12] uses convolutional followed by a GAP layer. Adds shortcut residual connection between convolutional layers.
- (11) Inception [13] is an ensemble of deep CNN models, inspired by the Inception-v4 architecture.

We normalize the datasets for each of our experiments. For datasets on which the accuracies of the baselines have been reported, we present the same results according to their papers. For the remaining datasets, we train all the baseline models with sufficient hyper-parameter tuning to produce results. Since our benchmark datasets are widely heterogeneous in terms of number of data points, features, sequence length, and sampling frequency, as well as the physical nature of the data itself, we obtain better performance via cursory tuning of architecture-specific hyper-parameters. To select hyper-parameters, we do a random 80%-20% split of the training set and used the 20% as a validation set for hyper-parameter tuning. After fixing the hyper-parameters, we train the model again using the entire training set and save the model with the lowest training loss. We use the saved model to evaluate on the official test set and report our evaluation metrics.

#### 4.2 Evaluation Metrics

We use accuracy and Root Mean Squared Error (RMSE) error as our performance metric for classification and regression, respectively. Considering the large number of datasets and baselines used, it is highly unlikely for a single model to outperform all other methods on every datasets. Therefore, we also present some summary statistics to present a holistic and a fairer comparison of the methods. The evaluation metrics are as follows:

- Ours 1-to-1 Wins/Draws/Losses: Number of datasets for which TARNet's accuracy or RMSE is better/same/worse than the corresponding baselines, respectively. Higher wins, lower draws and lower losses are better. This is useful to draw a one-on-one comparison between TARNet and a given model.
- Mean Rank: Average rank of a model across all datasets. Lowest rank is assigned to model with highest accuracy for classification and lowest RMSE for regression. Lower mean rank is better.
- Avg.Rel.Diff.Mean [37]: We report the "average relative difference from mean" metric  $r_j$  for each model j, over N datasets:

$$r_j = \frac{1}{N} \sum_{i=1}^{N} \frac{R(i,j) - \bar{R}_i}{\bar{R}_i}, \qquad \bar{R}_i = \frac{1}{M} \sum_{j=1}^{M} R(i,j), \qquad (8)$$

where R(i, j) is the RMSE of model j on dataset i and M is the number of models.  $r_j = -0.3$  means that the model on average attains 30% lower RMSE on a dataset than the average model performance on the same dataset. Lower value is better.

#### 4.3 Classification

Table 1 shows the accuracy of the models. According to Table 1, the overall accuracy of TARNet is the best among all compared methods. TARNet performs the best on 17 datasets, as compared to 7 and 6 by the next best baselines TST [37] and Rocket [5], respectively. TARNet achieves a 2.7-point higher average accuracy across all

Table 1: Accuracy of TARNet and baselines on classification datasets from UEA ARCHIVE and UCI MACHINE LEARNING REPOSITORY. We mark the best and <u>second best</u> values. Baselines are presented in ascending order (left to right) by average accuracy. A dash indicates that the corresponding method failed to run on this dataset. Higher Total best accuracy, average accuracy, and Ours 1-to-1 Wins is better. Lower Ours 1-to-1 Draws, Ours 1-to-1 Losses, and Mean Rank is better.

Dataset	ED	MLSTM-FC	Ns DTWD	TapNet	DTWI	NS	WEASEL-MUSE	e ts-tcc	TNC S	ShapeNet	TS2Vec	Rocket	MiniRocket	TST	TARNet
ArticularyWordRecognition	0.970	0.973	0.987	0.987	0.980	0.987	0.990	0.953	0.973	0.987	0.987	0.993	0.993	0.947	0.977
AtrialFibrillation	0.267	0.267	0.220	0.333	0.267	0.133	0.333	0.267	0.133	0.400	0.200	0.067	0.133	0.533	1.000
BasicMotions	0.676	0.950	0.975	1.000	1.000	1.000	1.000	1.000	0.975	1.000	0.975	1.000	1.000	0.925	1.000
CharacterTrajectories	0.964	0.985	0.989	0.997	0.969	0.994	0.990	0.985	0.967	0.980	0.995	0.991	0.990	0.971	0.994
Cricket	0.944	0.917	1.000	0.958	0.986	0.986	1.000	0.917	0.958	0.986	0.972	1.000	0.986	0.847	1.000
DuckDuckGeese	0.275	0.675	0.600	0.575	0.550	0.675	0.575	0.380	0.460	0.725	0.680	0.500	0.750	0.300	0.750
EigenWorms	0.549	0.504	0.618	0.489	-	0.878	0.890	0.779	0.840	0.878	0.847	0.650	0.790	0.720	0.420
Epilepsy	0.666	0.761	0.964	0.971	0.978	0.957	1.000	0.957	0.957	0.987	0.964	0.986	1.000	0.775	1.000
ERing	0.133	0.133	0.133	0.133	0.133	0.133	0.133	0.904	0.852	0.133	0.874	0.989	0.974	0.930	0.919
EthanolConcentration	0.293	0.373	0.323	0.323	0.304	0.236	0.430	0.285	0.297	0.312	0.308	0.450	0.430	0.337	0.323
FaceDetection	0.519	0.545	0.529	0.556	-	0.528	0.545	0.544	0.536	0.602	0.501	0.638	0.612	0.625	0.641
FingerMovements	0.550	0.580	0.530	0.530	0.520	0.540	0.490	0.460	0.470	0.580	0.480	0.520	0.550	0.590	0.620
HandMovementDirection	0.278	0.365	0.231	0.378	0.306	0.270	0.365	0.243	0.324	0.338	0.338	0.486	0.392	0.675	0.392
Handwriting	0.200	0.286	0.286	0.357	0.316	0.533	0.605	0.498	0.249	0.451	0.515	0.596	0.520	0.359	0.281
Heartbeat	0.619	0.663	0.717	0.751	0.658	0.737	0.727	0.751	0.746	0.756	0.683	0.741	0.771	0.782	0.780
InsectWingbeat	0.128	0.167	-	0.208	-	0.160	-	0.264	0.469	0.250	0.466	0.179	0.229	0.687	0.137
JapaneseVowels	0.924	0.976	0.949	0.965	0.959	0.989	0.973	0.930	0.978	0.984	0.984	0.978	0.986	0.995	0.992
Libras	0.833	0.856	0.870	0.850	0.894	0.867	0.878	0.822	0.817	0.856	0.867	0.906	0.922	0.861	1.000
LSST	0.456	0.373	0.551	0.568	0.575	0.558	0.590	0.474	0.595	0.590	0.537	0.635	0.653	0.576	0.976
MotorImagery	0.510	0.510	0.500	0.590	-	0.540	0.500	0.610	0.500	0.610	0.510	0.460	0.610	0.610	0.630
NATOPS	0.850	0.889	0.883	0.939	0.850	0.944	0.870	0.822	0.911	0.883	0.928	0.872	0.933	0.939	0.911
PEMS-SF	0.705	0.699	0.711	0.751	0.734	0.688	-	0.734	0.699	0.751	0.682	0.832	0.809	0.930	0.936
PenDigits	0.973	0.978	0.977	0.980	0.939	0.983	0.948	0.974	0.979	0.977	0.989	0.981	0.967	0.981	0.976
Phoneme			0.151	0.175	0.151	0.246	0.190	0.252	0.207	0.298	0.233	0.273	0.291	0.111	0.165
RacketSports	0.868	0.803	0.803	0.868	0.842	0.862	0.934	0.816	0.776	0.882	0.855	0.901	0.868	0.796	0.987
SelfRegulationSCP1	0.771	0.874	0.775	0.652	0.765	0.846	0.710	0.823	0.799	0.782	0.812	0.867	0.915	0.961	0.816
SelfRegulationSCP2	0.483	0.472	0.539	0.550	0.533	0.556	0.460	0.533	0.550	0.578	0.578	0.555	0.506	0.604	0.622
SpokenArabicDigits	0.967	0.990	0.963	0.983	0.959	0.956	0.982	0.970	0.934	0.975	0.988	0.997	0.963	0.998	0.985
StandWalkJump	0.200	0.067	0.200	0.400	0.333	0.400	0.333	0.333	0.400	0.533	0.467	0.467	0.333	0.600	0.533
UWaveGestureLibrary	0.881	0.891	0.903	0.894	0.868	0.884	0.916	0.753	0.759	0.906	0.906	0.931	0.785	0.913	0.878
PAMAP2	0.718	0.949	0.683	0.865	0.769	0.885	0.928	0.942	0.938	0.948	0.941	0.931	0.962	0.948	0.974
OpportunityGestures			0.762	0.574	0.715	0.689	0.553	0.791	0.821	0.730	0.771	0.813	0.809	0.732	0.830
OpportunityLocomotion			0.859	0.850	0.868	0.859	0.634	0.881	0.874	0.874	0.842	0.875	0.886	0.907	0.908
Occupancy [15]			0.517	0.844	0.526		0.556	0.865	0.828	0.852	0.876	0.832	0.878	0.881	0.883
Total best accuracy		0	1	2	1	2	5	1	0	2	1	6	4	7	17
Average accuracy		0.651	0.658	0.672	0.675	0.686	0.688	0.692	0.693	0.717	0.722	0.732	0.741	0.745	0.772
Ours 1-to-1 Wins		26	27	23	31	23	25	28	29	25	24	20	21	20	-
Ours 1-to-1 Draws	0	0	2	2	1	2	3	1	1	2	0	2	4	0	-
Ours 1-to-1 Losses	2	8	5	9	2	9	6	5	4	7	10	12	9	14	-
Mean Rank			9.65	7.44	10.44	7.59	7.79	9.03	9.41	5.47	7.18	5.18	4.71	5.74	4.00

datasets over TST. The closest competitors of TARNet are TST and Rocket, but TARNet still outperforms them on 20 datasets while losing on 14 and 12, respectively. TARNet ranks 1<sup>st</sup> (lowest "Mean Rank") on average, having a 0.71-point lower average than the 2<sup>nd</sup> best MiniRocket. Rocket and ShapeNet ranks 3<sup>rd</sup> and 4<sup>th</sup> with a 1.18 and 1.47-point higher average, respectively, than TARNet.

The large number of datasets and baselines used makes it highly unlikely for a single model to outperform all other methods on every dataset. For example, TST had the 2<sup>nd</sup> best "Total best Accuracy" (7) and "Average Accuracy" (0.745), but it ranks 5<sup>th</sup> across all models, with a 1.74-point higher average than TARNet. This means that for the datasets where TST under-performs, its performance metrics are significantly below those of other baselines, pushing down its "Mean Rank." However, TARNet performs well across all evaluation metrics. Not only does it have the highest "Total best Accuracy" (17) and "Average Accuracy" (0.772), but it also ranks 1<sup>st</sup>, meaning that for the datasets where TARNet under-performs, it still generates better performance than most of its baselines, pushing up its "Mean Rank". Moreover, from Table 1, we find that on datasets where TARNet under-performs, the winning methods are in fact different. Considering that no single baseline is consistently better than TARNet, as illustrated by the baselines' low number of best accuracies, low average accuracies and high mean rank, we argue that TARNet is the new benchmark for time-series classification.

Moreover, TARNet achieves the best accuracy across a diverse set of data characteristics. For example, TARNet has the best accuracy for Atrial Fibrillation and Occupancy with 15 and 1.2*m*+ training data points, respectively, for RacketSports and Cricket with sequence length of 30 and 1197, respectively, for Epilepsy and FaceDetection with 3 and 44 features, respectively and for MotorImagery and OpportunityGestures with 2 and 17 classes, respectively.

#### 4.4 Regression

We compare regression results against all the baselines reported by TST [37]. Table 2 shows the Root Mean Squared Error of the models. TARNet ranks 1<sup>st</sup> on three and 2<sup>nd</sup> on two datasets, which

Table 2: Root Mean Squared Error (RMSE) Performance of TARNet and baselines on regression datasets from MONASH UNIVER-SITY, UEA, UCR TIME SERIES REGRESSION ARCHIVE [27]. We mark the best and <u>second best</u> values. Baselines are presented in descending order (left to right) by mean rank. Avg.Rel.Diff.Mean: Average Relative Difference from Mean over all models, e.g. -0.3 means that the model on average attains 30% lower RMSE than the average model performance. Higher Total best loss and Ours 1-to-1 Wins is better. Lower Ours 1-to-1 Draws, Ours 1-to-1 Losses, Mean Rank, and Avg.Rel.Diff.Mean is better.

Dataset	1-NN-DTWD	1-NN-ED	5-NN-ED	5-NN-DTWD	SVR	ResNet	FCN	Rocket	Inception	RF	XGB	TST	TARNet
AppliancesEnergy	6.036	5.231	4.227	4.019	3.457	3.065	2.865	2.299	4.435	3.455	3.489	2.375	2.173
BenzeneConcentration	4.983	6.535	5.844	4.868	4.790	4.061	4.988	3.360	1.584	0.855	0.637	0.494	0.481
BeijingPM10	139.134	139.229	115.502	115.502	110.574	95.489	94.438	120.057	96.749	94.072	93.138	86.866	90.482
BeijingPM25	88.256	88.193	74.156	72.717	75.734	64.462	59.726	62.769	62.227	63.301	59.495	53.492	60.271
LiveFuelMoisture	57.111	58.238	46.331	46.290	43.021	51.632	47.877	41.829	51.539	44.657	44.295	43.138	41.091
IEEEPPG	37.140	33.208	27.111	33.572	36.301	33.150	34.325	36.515	23.903	32.109	31.487	27.806	26.372
Total best loss	0	0	0	0	0	0	0	0	1	0	0	2	3
Ours 1-to-1 Wins	6	6	6	6	6	6	5	6	5	6	5	4	-
Ours 1-to-1 Draws	0	0	0	0	0	0	0	0	0	0	0	0	-
Ours 1-to-1 Losses	0	0	0	0	0	0	1	0	1	0	1	2	-
Mean Rank	12.167	11.833	8.833	8.833	8.000	7.333	7.000	6.500	6.500	5.500	4.333	2.500	1.833
Avg.Rel.Diff.Mean	0.355	0.379	0.153	0.125	0.097	0.006	0.022	-0.047	-0.107	-0.171	-0.196	-0.302	-0.313

**Table 3: Ablation study of TARNet** 

	TARNet-Random	TARNet-Top $\mu$	TARNet						
	Results on 34 classification datasets								
Total best accuracy	6	<u>9</u>	31						
Average accuracy	0.752	0.741	0.772						
Ours 1-to-1 Wins	28	25	-						
Ours 1-to-1 Draws	5	7	-						
Ours 1-to-1 Losses	1	2	-						
Mean Rank	2.206	2.176	1.088						
	Results on 6 regression datasets								
Total best loss	0	1	5						
Ours 1-to-1 Wins	6	5	-						
Ours 1-to-1 Draws	0	0	-						
Ours 1-to-1 Losses	0	1	-						
Mean Rank	2.667	2.167	1.167						
Avg.Rel.Diff.Mean	0.046	0.014	-0.060						

is better than what any of the baseline models achieve. For the overall rank, TARNet achieves an average rank of 1.833, setting it clearly apart from all other models; the overall second best model, TST [37] has an average rank of 2.5; XGB, Inception, and FCN (which outperformed TARNet on one dataset) on average ranks 4.333, 6.5, and 7, respectively. Both TST [37] and TARNet use a similar transformer backbone model which explains the small difference in Avg.Rel.Diff.Mean scores. However, TARNet still outperforms TST and all other baseline models by attaining 31.3% lower RMSE on average than the mean RMSE among all models. Considering that TARNet achieves the highest number of best losses, lowest mean rank, and lowest Avg.Rel.Diff.Mean in Table 2, we argue that TARNet is the new benchmark for time-series regression.

Although TST [37] pretrains and finetunes on the same dataset, the data reconstruction and the supervised end-task runs *sequentially*, slowing down training time. However, TARNet trains both tasks,  $T_{TAR}$  and  $T_{END}$  parallely. Hence, not only TARNet outperforms TST on the end-task but it also trains faster than TST.

#### 4.5 Ablation Study

We justify our design choices of M through ablation study results on classification and regression tasks in Table 3. TARNet-Random uses the same architecture as TARNet but instead masks timestamps

randomly and reconstructs them, giving substandard performance. TARNet-Top  $\mu$  selects timestamps corresponding to the top  $\lfloor \mu S \rfloor$  values in  $\sigma$  and masks them from X for reconstruction. This does not lead to a clear improvement which may be attributed to *overfitting*, as explained in Section 3.5. This prompts sampling to TARNet-Top  $\mu$  while selecting the timestamps to mask from the set of important timestamps, resulting in TARNet. To ensure a fair comparison, we maintain the same set of hyper-parameters across all ablation models for each dataset. Table 3 shows that TARNet has the highest average accuracy, most number of datasets with highest accuracy and lowest loss, and lowest mean rank. TARNet combines ideas from both TARNet-Random and TARNet-Top  $\mu$  to counter their individual drawbacks and yields better performance.

# 4.6 Can *T<sub>TAR</sub>* compensate for limited labeled training data?

We study whether under data-deficient environments TARNet can make better use of limited data compared to baselines. This will illustrate if the knowledge gained during reconstruction,  $T_{TAR}$ , can compensate for a lack of labeled data to train the end task,  $T_{END}$ .

We choose occupancy and human gestures datasets for classification. As Figure 2 (a) and (b) show, the accuracy of all models increases as the amount of training data increases. Particularly, TARNet has a steep rise for both datasets, signifying that the greatest improvement occurs with low quantity of training data. Similarly, we choose LiveFuelMoisture and IEEEPPG datasets for regression. As Figure 2 (c) and (d) show, the RMSE Loss of all models decreases as the amount of training data increases. Even with just 25% training data, TARNet achieves significantly lower loss than any baselines. It achieves superior performance over all baselines at all quantities of training data, for both classification and regression.

Both TST and TARNet can leverage additional information learnt though reconstruction to compensate for the lack of labeled data, resulting in better performance over other baselines. However, making the reconstruction task-aware improves the performance of TARNet over TST. For example, in Occupancy, TARNet achieves the same performance with 50% training data, which TST and ShapeNet require 75% training data to achieve. Similarly, for LiveFuelMoisture KDD '22, August 14-18, 2022, Washington, DC, USA

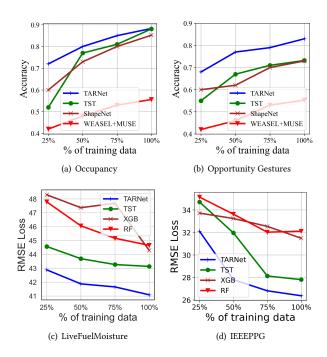


Figure 2: (a) and (b) show classification accuracy, and (c) and (d) show regression RMSE Loss against % of training data.

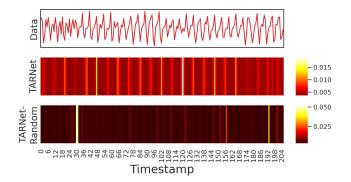


Figure 3:  $\sigma$  plotted as heatmap for Epilepsy.

and IEEEPPG, TARNet achieves lower RMSE with just 25% and 50% training data, respectively, than TST does with 100% training data.

#### 4.7 Explaining Masking Strategy, M

We provide two real-world case studies to show why a task-aware reconstruction learnt through a data-driven masking strategy, M, is superior to a reconstruction learnt through random masking. For qualitative analysis, we show normalized aggregate attention,  $\sigma$ , computed from attention maps of Transformer during  $T_{END}$ .

**Case Study I: Epilepsy.** Figure 3 shows a time-series plot of an accelerometer data from a person conducting the activity of "Sawing" (classification label). Following the time-series plot are the  $\sigma$  scores, as discovered by TARNet and TARNet-Random. Sawing involves strong periodic motion of the hand as illustrated by the time-series plot. Figure 3 shows that a random-masking based auto-regressive task (TARNet-Random) could not capture this inherent

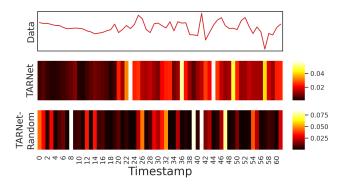


Figure 4:  $\sigma$  plotted as heatmap for Face Detection.

periodicity in the data, which TARNet could successfully decipher. Therefore, the accuracy achieved by TARNet and TARNet-Random is 1 and 0.75, respectively. Being able to selectively mask "important" timestamps during reconstruction in a data-driven manner enables TARNet to effectively capture the domain-specific properties from the data, leading to better classification performance.

Case Study II: Face Detection. A person is shown a face image or a scrambled image and her MEG readings are recorded. The task is to determine what the person saw (classification) based on the collected MEG data. The MEG recording (response) is collected over 1.5-second but the image (stimulus) is only shown 0.5-seconds after the MEG has started recording. Figure 4 shows the time-series plot of a sample MEG data. Since the entire 1.5-second corresponds to 62 timestamps, this means that no stimulus was provided to the subject for the first 20 timestamps (0.5-seconds). So the discriminatory MEG response, important for classification, is received from 20-th timestamp onward, as illustrated by the onset of sudden fluctuation in signal strength. Figure 4 shows that TARNet assigns high  $\sigma$  values around the 20-th timestamp and can clearly infer the signal arrival time from the MEG response. TARNet discriminates between the "unimportant" and "important" timestamps for classification by assigning higher average attention per timestamp for times greater than 20 than to those before 20. However, TARNet-Random fails to infer such task-specific domain properties from the data and assigns attention weights randomly across time. Hence, TARNet-Random achieves an accuracy of 0.607, whereas TARNet achieves 0.641.

The two case studies substantiate why using M to decide which timestamps to mask during reconstruction is important. Representations learnt through reconstructing "important" timestamps reflect some domain-specific inherent properties in the data, as illustrated by how the attention scores have been assigned. Such domain properties are relevant to the end task and can clearly lead to performance improvement on the end task, as illustrated in Table 1 and 2. We also highlight that the utility of self-attention goes beyond computing internal data representation of a model to improve performance [29] or providing meaningful explanations [17, 34]. In addition, self-attention can also be used to integrate simple and intuitive data-driven techniques into deep learning frameworks.

#### 5 DISCUSSION AND CONCLUSIONS

We have proposed a task-aware reconstruction technique to improve end-task performance for a time series. In particular, we use

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attention score distribution to identify timestamps important to an end task. We then sample from those important timestamps and mask them from the data for reconstruction, making the reconstruction *end task-aware*. These tasks are trained alternately, sharing parameters in the same model, thereby enabling the representation learnt through reconstruction to improve end-task performance. Experimental results show that TARNet outperforms the state-ofthe-art baselines for both classification and regression tasks. The ablation study highlights the essence of our design choices for the data masking technique, and the case study observations show how TARNet captures the intrinsic task-specific properties of data.

Additional unlabeled data can help to improve TARNet. Although the data reconstruction task is fully unsupervised, it is driven by the end task that requires labeled data. In the future, we wish to explore such task-aware representations under data shift problem and in the presence of outliers.

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