PrimeNet: Pre-training for Irregular Multivariate Time Series

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Abstract

Real-world applications often involve irregular time series, for which the time intervals between successive observations are non-uniform. Irregularity across multiple features in a multi-variate time series further results in a different subset of features at any given time (i.e., asynchronicity). Existing pre-training schemes for time-series, however, often assume regularity of time series and make no special treatment of irregularity. We argue that such irregularity offers insight about domain property of the data—for example, frequency of hospital visits may signal patient health condition—that can guide representation learning. In this work, we propose PrimeNet to learn a self-supervised representation for irregular multivariate time-series. Specifically, we design a time-sensitive contrastive learning and data reconstruction task to pre-train a model. Irregular time-series exhibits considerable variations in sampling density over time. Hence, our triplet generation strategy follows the density of the original data points, preserving its native irregularity. Moreover, the sampling density variation over time makes data reconstruction difficult for different regions. Therefore, we design a data masking technique that always masks a constant time duration to accommodate reconstruction for regions of different sampling density. We learn with these tasks using unlabeled data to build a pre-trained model and fine-tune on a downstream task with limited labeled data, in contrast with existing fully supervised approach for irregular time-series, requiring large amounts of labeled data. Experiment results show that PrimeNet significantly outperforms state-of-the-art methods on naturally irregular and asynchronous data from Healthcare and IoT applications for several downstream tasks, including classification, interpolation, and regression.

Introduction

Many real-world applications generate data with non-uniform time-interval between successive observations. For example, sensors are triggered at irregular intervals driven by events in real-life. Further, not all sensors are triggered at the same time. Thus, irregularity (in time) and asynchronicity (across sensors) are natural characteristics of many time series that provide rich insights into real-world events. Naturally occurring irregularity in many datasets reflect intrinsic domain property about the underlying system, which can be leveraged to learn the task better. For example, to predict whether a patient is sick or healthy based on their schedule of doctor visits and medical test results, the frequency of visits may be a useful signal, in addition to the physiological variables, i.e., sick patients visit doctors more frequently than healthy ones. However, no regular time series models, whether fully- (Chowdhury et al. 2022), semi- (Zerveas et al. 2021) or un- (Tonekaboni, Eytan, and Goldenberg 2021) supervised, encode time information. They assume constant time intervals between all consecutive observations in a sequence (regularity) with all features observed at any given time (synchronicity) (Marlin et al. 2012). Hence, simply adapting pre-trained regular time-series methods for irregular time-series is sub-optimal.

Recently, ODE- (Rubanova, Chen, and Duvenaud 2019), attention- (Shukla and Marlin 2021), and set- (Horn et al. 2020) based models that directly learn time information and encode irregularity have outperformed regular time series models on irregular data. However, most of these irregular methods are fully- (Rubanova, Chen, and Duvenaud 2019) or semi- (Shukla and Marlin 2021) supervised, requiring large amounts of labeled data. Data labeling in IoT is time-consuming and both cost and labor-intensive as it involves physical sensor deployment and human annotators with domain expertise. Moreover, accessing labeled data in healthcare may raise security and privacy concerns.

To this end, we propose PrimeNet, the first pre-trained model for irregular multivariate time series. Specifically, we design two time-sensitive tasks based on contrastive learning and data reconstruction to build a self-supervised representation from completely unlabeled irregular time series data. Time-slicing (Franceschi, Dieuleveut, and Jaggi 2019), which chunks a time series into slices containing equal number of readings, is commonly used to augment regular time-series data for contrastive learning. However, it cannot generate representative sub-sequences for an irregular time series as irregular time series exhibit significant variations in sampling density over time and the sampling density of a given time slice may not mirror that of the entire time series (Figure 3). A common approach would be to randomly sample observations from an irregular time series to construct a sub-sequence. However, an irregular time series may also exhibit significant imbalanced occurrences of dense and sparse observations. Hence, random sampling will lead to
Related Work

Self-Supervised Regular Time Series Methods

Recent research on learning unsupervised representations from regular and synchronous time-series performs well under limited labeled data settings, using triplet loss (Franceschi, Dieuleveut, and Jaggi 2019), hierarchical contrastive loss (Yue et al. 2021; Chowdhury, Adnan, and Gupta 2020), Fourier transform (Li et al. 2021; Zhang et al. 2023), task-aware reconstruction (Chowdhury et al. 2022). They can be adapted to irregular time-series by discretizing continuous-time samples into uniformly-spaced fixed-size bins (Shukla and Marlin 2019; Zhang et al. 2022). However, irregular time series are marked by regions of high and low sampling densities. A wide bin would aggregate data in dense regions, resulting in a loss of fine-grained details. A short bin would generate a high fraction of missing data in sparse regions exploding the sequence length, making imputation increasingly difficult. Consequently, imputation-based methods are hardly used to learn from such irregular time series. Moreover, by treating irregular time series data like a regular one, they abstract the vital irregular time information away from the model, inhibiting performance.
We exploit the irregular time-interval property to design our self-supervision tasks to pre-train PrimeNet, thereby learning suitable representations from unlabeled irregular and asynchronous multivariate time-series data.

Irregular Time Series Methods

Gated Recurrent Unit (GRU)-based methods (Che et al. 2018) involve modifying the LSTM forget gate (Pham et al. 2017) or introducing new time gate (Neil, Pfeiffer, and Liu 2016). (Chen et al. 2018) combined a neural network with a latent ordinary differential equation (ODE) model. (Rubanova, Chen, and Duvenaud 2019; Lechner and Hasani 2020) used neural ODEs to model hidden state dynamics. Others use attention mechanism (Zhang 2019; Tan et al. 2020) similar to (Vaswani et al. 2017) by replacing positional encoding with a fixed time encoding. (Shukla and Marlin 2021) learns time representation. Marlin 2021; Kazemi et al. 2019) learns time representation. We present PrimeNet’s core architecture - Time Embedding, Time-Feature Attention (TFA) and Feature-Feature Attention (FFA), as shown in Figure 4.

Notation

An individual data case is a $N$-dimensional, irregularly and asynchronously sampled multivariate time series, $D = (T, X, M)$, where $T \in \mathbb{R}^S$, $X \in \mathbb{R}^{S \times N}$, and $M \in \mathbb{R}^{S \times N}$. $T$ denotes the union of timestamps at which all the $N$ features have been sampled and $S$ is the number of such timestamps. Let $t$ and $n$ represent a particular time and feature, respectively, in $D$. $X \in \mathbb{R}^N$ represents the feature values sampled at time $t$. This formulation also covers the uni-variate case when $N = 1$. However, since the time-series is asynchronously sampled, not all the $N$ features may be sampled at $t$. Hence, we use masking variable $M \in \mathbb{R}^N$ to denote the set of observed features. Specifically, $M_n \in \mathbb{R}^N$ denote the set of observed and unobserved features at $t$. If feature $n$ is sampled at $t$, then $M_{tn} = 1$, otherwise $M_{tn} = 0$. Using $M$ to deal with unobserved dimensions allows us to transform the irregular length time-series into uniform length and parallelize computations, thereby enabling efficient GPU implementation.

Our time-sensitive self-supervision tasks are model agnostic and can be plugged into any irregular time series architectures, like ODE-, attention-, or set-based models, that explicitly encode time information. We follow a similar architecture to mTAND (Shukla and Marlin 2021) because it is the current state-of-the-art for irregular time series. Our model is pre-trained on unlabeled data using time-sensitive contrastive and data reconstruction loss and then fine-tuned on available labeled data for a given downstream task.

Model Architecture

We present PrimeNet’s core architecture - Time Embedding, Time-Feature Attention (TFA) and Feature-Feature Attention (FFA), as shown in Figure 4.

Time Embedding (Shukla and Marlin 2021) embeds continuous time points into a vector space by leveraging $H$ embedding functions $\phi h(T)$, each outputting a representation of size $d_r$. Dimension $i$ of embedding $h$ is defined as:

$$\phi h(T)[i] = \begin{cases} 
\omega_{ih} T + \alpha_{ih}, & \text{if } i = 0 \\
\sin(\omega_{ih} T + \alpha_{ih}), & \text{if } 0 < i < d_r 
\end{cases} \quad (1)$$

where $\omega_{ih}$’s and $\alpha_{ih}$’s are learnable parameters. Linear term encodes the non-periodic patterns. Periodic terms captures periodicity with $\omega_{ih}$ and $\alpha_{ih}$ as frequency and phase.

Time-Feature Attention, TFA (Shukla and Marlin 2021) captures the interaction between feature values with their corresponding sampling times. The output from the Time Embedding layer forms the query $Q_T$ and key $K_T$ vectors.

$$\text{TFA}(Q_T, K_T, M, X) = (M \odot A_T) X, \quad A_T = \text{softmax}(Q_T K_T / d_r) \quad (2)$$

We do an element-wise multiplication of $M$ with $A_T$ to nullify the effect of unobserved features in $X$ at a given sampling time in $T$. We compute a weighted summation of features, where weights are self-attention scores of features’ corresponding sampling time embeddings, $Q_T$ and $K_T$.

Feature-Feature Attention, FFA (Vaswani et al. 2017) models the self-attention within features. The output from TFA becomes the query, key and value vectors for FFA.

$$Q_X = K_X = V_X = \text{TFA}(Q_T, K_T, M, X) \quad (3)$$

Then, FFA will encode the outputs from TFA as follows:

$$\text{FFA}(Q_X, K_X, V_X, M) = (M \odot A)V_X, \quad A = \text{softmax}(Q_X K_X / d_r) \quad (4)$$

The output of FFA is fed through residual and feed forward layers like in a typical Transformer Encoder. The data is fed through $N$ such Encoders to generate the output $X$.

Time-Sensitive Pre-training

We present two time-sensitive self-supervised pre-training objectives, namely, Time Contrastive Learning (TimeCL) and Time Reconstruction (TimeReco). We discuss how we augment the data, followed by loss computation details.

Time Contrastive Learning (TimeCL)

Augmenting data for contrastive learning through time-slicing or random sampling fails to capture the irregularity in data, motivating our stratified-sampling based approach.
Algorithm 1: TimeCL Data Augmentation

**Input:** \( D \)

**Hyper-parameters:** \((\mu_1, \mu_2), (\lambda_1, \lambda_2)\)

**Output:** \(D_A, D_P\)

1. \( Z \leftarrow \{ (T_i - T_{i+1}) / 2 \}_{i \in \mathbb{Z}^+} \times \{ T_{i+1} - T_i \}_{i \in \mathbb{Z}^+}, 1 < i < S \}, Z \in \mathbb{R}^S \)
2. Sort \((Z, T)\) in ascending order of \( Z \)
3. \( T_{\text{dense}} \leftarrow T[1 : S/2], T_{\text{dense}} \in \mathbb{R}^{S/2} \)
4. \( T_{\text{sparse}} \leftarrow T[S/2 : S], T_{\text{sparse}} \in \mathbb{R}^{S/2} \)
5. \( \mu \sim \mathcal{U}(\mu_1, \mu_2), 0 < \mu_1 < \mu_2 < 1 \)
6. \( \lambda \sim \mathcal{U}(\lambda_1, \lambda_2), 0 < \lambda_1 < \lambda_2 < 1 \)
7. \( T_A \sim \text{Sample} \lambda \mu S \) and \((1 - \lambda) \mu S \) timestamps from \( T_{\text{dense}} \) and \( T_{\text{sparse}} \), respectively, \( T_A \in \mathbb{R}^{\mu S} \)
8. \( T_P \leftarrow T - T_A, T_P \in \mathbb{R}^{(1-\mu)S} \)
9. \( D_A, D_P \leftarrow (T_A, X_{T_A}, M_{T_A}), (T_P, X_{T_P}, M_{T_P}) \)
10. **return** \(D_A, D_P\)

**Data Augmentation**

Contrastive learning (Chen et al. 2020; Hogan, Li, and Shang 2022) augments observations from the same input to form an anchor and positive (similar to anchor), while a sample from other in-batch inputs form the negative (different from anchor). This pulls the latent space of the anchor and positive closer while pushing away the negatives, learning good data representation (Jaiswal et al. 2020; Li, Shang, and McAuley 2022).

To better replicate the irregularity pattern of data, we maintain an approximate sampling density distribution of the data in its augmented sub-sequences, as outlined in Algorithm 1. For every sampling time \( T_i \), we compute its mean time interval, \( Z_i \), by averaging the time lapse between its immediate predecessor, \( T_{i-1} \), and successor, \( T_{i+1} \), to estimate the local density of the sampled features at \( T_i \) (Line 1). We reorder \( Z \) and \( T \) in ascending order of \( Z \) and group \( T \) into two bins, \( T_{\text{dense}} \) (lowest 50% Z-values) and \( T_{\text{sparse}} \) (highest 50% Z-values) (Lines 2 - 4). We sample a proportion of the timestamps from \( T_{\text{dense}} \) and the remaining from \( T_{\text{sparse}} \) to form the sampled timestamps of one augmented sub-sequence, \( T_A \) (Line 6). The remaining \( T - T_A \) timestamps form the sampled timestamps of the other sub-sequence, \( T_P \) (Line 8). This stratified sampling technique ensures that we draw observations from regions of different sampling density of \( D \), regardless of how scarce the observations from certain regions are. Hence, the augmented sub-sequence can better approximate the irregularity in \( D \). To preserve asynchronicity of \( D \), we extract only the subset of features that was sampled together at a given time in \( D \) to form the feature set for that time in the augmented sub-sequence. Thus, \( D_A = (T_A, X_{T_A}, M_{T_A}) \) and \( D_P = (T_P, X_{T_P}, M_{T_P}) \) form good quality anchor and positive sub-sequences, respectively, that are representative of \( D \), thereby improving contrastive learning.

**Contrastive Loss, \( \mathcal{L}_{CL} \)**

For a given \( X_A \) and \( X_P \), the \( X_N \) is formed from all other instances in the same mini-batch. We add a special \([CLS]\) symbol in front of every input and pass it through an embedding layer. The final hidden state corresponding to \([CLS]\) is used as the aggregate sequence representation for contrastive learning.

We use Normalized Temperature-scaled Cross Entropy (NT-Xent) Loss (Chen et al. 2020) as our Contrastive Loss function. This has shown improvement over other contrastive losses, like CPC (Oord, Li, and Vinyals 2018) and MoCo (He et al. 2020), in several other domains (Chen et al. 2020). It is a modification of the multi-class \( B \)-pair loss, where \( B \) is the batch size, with addition of the temperature parameter, \( \tau \), to scale the cosine similarities as follows:

\[
\mathcal{L}_{CL} = -\log \frac{\exp(\tilde{X}_i \tilde{X}_j / \tau)}{\sum_k^B \exp(\tilde{X}_i \tilde{X}_k / \tau)}
\]

**Time Reconstruction (TimeReco)**

Masking constant length of data across time is not suitable to learn reconstruction from non-uniform time-interval data, prompting a constant time masking technique.

**Data Augmentation**

Reconstruction for irregular time-series presents two key challenges. First, some regions are more densely sampled than others. Therefore, masking a constant length of data will mask over a shorter time-interval for a denser region compared to a sparser region, as shown in Figure 2(b). Hence, reconstructing data at the masked segment may be trivial for the dense region with abundant contextual information but difficult for a sparse region. Second, for multivariate time-series, each feature may have different sampling frequency and may be sampled over different duration. Hence, each feature has different time gaps between successive observations, i.e. asynchronicity, rendering a constant length masking strategy ineffective.

To learn a better reconstruction for irregular time-series, we propose Algorithm 2. We specify the number of masking segments \( J \), and the fraction of time interval \( \alpha \), to mask for each segment. To address the asynchronicity problem, we compute the timespan \( q_n \), to mask separately for each feature \( n \) (Line 5) because the total duration for which each feature
lasts may vary. Features lasting shorter should have shorter masking segments as compared to those lasting longer. To deal with irregularity within a time-series, we fix the timespan \( q_n \) to mask for feature \( n \), instead of fixing the number of observations to mask. This adapts the length of masking segment based on the sampling density of the time-series in the masking region, as shown in Figure 2(c). For a given \( q_n \), a dense region will mask more observations than a sparse region. Hence for denser regions, there will not be sufficient unmasked observations in close temporal proximity of the masked segment to make the reconstruction trivial. Similarly for sparser regions, the number of masked observations will be low, so there will be sufficient observations in the temporal vicinity of the masked region to keep the task tractable. Lines 6 - 10 outlines this procedure.

Reconstruction Loss, \( \mathcal{L}_{\text{Reco}} \) We feed the masked out features \( \tilde{X}_U \) to PrimeNet and extract the generated features \( \tilde{X}_V \). The Reconstruction Error between model output \( \tilde{X}_U \) and target \( X_V \), is computed using Mean Squared Error (MSE),

\[
\mathcal{L}_{\text{Reco}} = \left\| M_V \odot (\tilde{X}_U - X_V) \right\|_2^2
\]

Hence the total loss \( \mathcal{L} \) becomes:

\[
\mathcal{L} = \eta \mathcal{L}_{\text{CL}} + (1 - \eta) \mathcal{L}_{\text{Reco}},
\]

where \( \eta \) is a hyperparameter, \( 0 < \eta < 1 \). It balances the two losses because different datasets may benefit differently from these two tasks.

Figure 5(a) shows the pre-training workflow of PrimeNet. For a given data point \( D \), we feed it through Algorithm 1 to generate the anchor \( D_A \), and positive \( D_P \). Additionally, we feed \( D \) through Algorithm 2 to mask its features and prepare the masked input \( \tilde{D}_U \) and target \( D_V \).

For finetuning on supervised downstream tasks, like classification, regression and interpolation, we append task-specific layers on top of pre-trained PrimeNet, as shown in Figure 5(b). The task-specific layers typically consists of some fully connected layers with non-linear activation.

Experiments

We evaluate PrimeNet on some real-world irregular and asynchronous time-series data from Healthcare and IoT domain for classification, regression, and interpolation tasks.

Datasets

- PhysioNet Challenge 2012 (Silva et al. 2012) and MIMIC-III (Johnson et al. 2016) are multivariate time series datasets consisting of 37 and 12 physiological variables, respectively, extracted from intensive care unit (ICU) records. Each record contains 48 hours of measurements after admission to ICU. We predict in-hospital mortality (binary classification) from this data.
- Activity (Kaluža et al. 2010) dataset has 3-D positions of the waist, chest and ankles from 5 individuals performing activities including walking, sitting, lying, standing, etc.
- Appliances Energy (Tan et al. 2021) dataset contains 138 time series with 24 dimensions, including temperature, humidity, pressure, wind speed, visibility, and dew point. The data is averaged for 10 minutes and spans 4.5 months. PhysioNet, MIMIC-III, and Activity are naturally irregular, i.e., data was sampled at irregular times during collection. Appliances Energy is a regularly sampled dataset where we synthetically induce irregularity by dropping out random data. To better understand their irregularity pattern, we provide some summary statistics: (mean, standard deviation) of the missing ratio of each feature’s time series across the dataset. If a dataset was sampled for 100 timestamps, then a 0.75 mean missing ratio means that on average, each feature was present for 25% and was missing for the remaining 75 timestamps across this dataset. Missing ratio statistics: PhysioNet (0.86, 0.24), MIMIC-III (0.65, 0.36), Activity (0.75, 0.64), Appliances Energy (0.87, 0.47).

Baselines

Self-Supervised Regular Time-Series Methods

1. TS2Vec (Yue et al. 2021) performs hierarchical contrastive learning over augmented context views.
2. TNC (Tonekaboni, Eytan, and Goldenberg 2021) defines temporal neighborhoods from local smoothness of data.
3. TST (Zerveas et al. 2021) pre-trains Transformer by masking fixed length segments and reconstructing them.

Irregular Time-Series Methods

1. GRU-Mean (Che et al. 2018) combines hidden state decay with input decay.
2. P-LSTM (Neil, Pfeiffer, and Liu 2016) adds a learnable oscillator to modulate LSTM to create dependencies on elapsed-time, and uses vanishing factor in gradients.
3. RNN-VAE VAE model with RNN encoder and decoder.
4. ODE-RNN (Rubanova, Chen, and Duvenaud 2019) uses neural ODEs to model hidden state dynamics and RNN to update hidden states with new observations.
6. mTAND (Shukla and Marlin 2021) Multi-time attention module followed by a VAE-based encoder-decoder.
Experimental Protocols

We infer a continuous missing segment of 10% and 50% values for interpolation, while conditioning on the remaining 90% and 50% of the observed points for Activity and PhysioNet, respectively. For interpolation, we use the entire output representation from PrimeNet, while for classification and regression we use the final hidden state of [CLS] symbol as the aggregate sequence representation. We compute Cross-Entropy Loss for classification and Root Mean Squared Error (RMSE) for regression and interpolation. Due to class imbalance in Physionet and MIMIC-III, we assess classification using Area Under the ROC curve (AUC score). We assess interpolation and regression using RMSE.

During pretraining, we measure contrastive learning classification (i.e. how many samples are predicted correctly among the 2B sub-samples) and use the validation accuracy for early stopping. During finetuning, we update the parameters of both the task-specific layers and PrimeNet.

We conduct grid search on hyper-parameters, $\eta = (0.3, 0.4, 0.5, 0.6, 0.7)$, $\alpha = (0.15, 0.05, 0.03)$, $J = (1, 3, 5)$, $\mu_1, \lambda_1 = (0.3, 0.4)$ and $\mu_2, \lambda_2 = (0.7, 0.6)$ to report test results based on the best held-out validation performance. Best values for $\eta = 0.5, 0.6, 0.5, 0.5$ for PhysioNet, MIMIC-III, Activity, Appliances Energy, respectively.

Results

Table 1 and 2 show the results. $k$-shot refers to $k$ labeled training examples. For each few-shot setup, we repeat an experiment five times using a different training sample set each time, to report the mean and standard deviation of metrics. We mark the best and second best values.

Classification Table 1 shows AUC scores on mortality prediction task (binary classification) of PhysioNet and MIMIC-III datasets. For the fully supervised irregular time-series methods.
We propose a self-supervised representation learning approach to model irregular and asynchronous multivariate time-series. We use time-sensitive contrastive learning that preserves an approximate sampling density distribution of the data to learn from representative sub-sequences. We use time-sensitive data reconstruction to mask a fixed duration of data, instead of a fixed number of points, making reconstruction tractable across regions of varying sampling density. Our pre-trained model is then fine-tuned on downstream end tasks. Experiment results show that PrimeNet outperforms both fully- and semi-supervised irregular time-series and self-supervised regular time-series methods on classification, interpolation and regression tasks across several real-world datasets. In future, we plan to apply this to irregular time-series forecasting and unsupervised anomaly detection.
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