What went wrong and when?
Instance-wise Feature Importance for Time-series Models

Abstract
Multivariate time series models are poised to be used for decision support in high-stakes applications, such as healthcare. In these contexts, it is important to know which features at which times most influenced a prediction. We demonstrate a general approach for assigning importance to observations in multivariate time series, based on their counterfactual influence on future predictions. Specifically, we define the importance of an observation as the change in the predictive distribution, had the observation not been seen. We integrate over plausible counterfactuals by sampling from the corresponding conditional distributions of generative time series models. We compare our importance metric to gradient-based explanations, attention mechanisms, and other baselines in simulated and clinical ICU data, and show that our approach generates the most precise explanations. Our method is inexpensive, model agnostic, and can be used with arbitrarily complex time series models and predictors.

1. Introduction
In high-stakes applications such as healthcare, explaining the model outcome is crucial to build trust with end-users (Tonekaboni et al., 2019). Clinicians would like to understand which patient measurement and at what point in time, most influenced the model prediction. Explaining time series model predictions is challenging due to complex non-linear temporal dependencies in the data. To explain time series models, it is not sufficient to identify important features driving the outcome. We additionally need to identify critical points in time where a change in the signal had a significant effect on the downstream outcome. That is, explanation of time series data needs to capture changes in the importance of features over time. Changes in patients dynamics are often more informative than the actual measurements. Thus explaining model outcome by evaluating changes in feature importance can allow clinicians to intervene differently (Schneider, 2019).

Most feature importance attribution methods in time series have focused on population level importance (Yang et al., 2005; Yoon et al., 2005; Hmamouche et al., 2017). Population level feature importance may not characterize local explanations reliably for individual samples, especially in heterogeneous populations. Such explanations are not helpful for users trying to understand model outcome for specific cases. Our work focuses on instance-level feature importance in time series settings. In particular, we propose Feature Importance for Time-series (FIT) as a model agnostic approach for assigning the importance of observations in a multivariate time series. We measure the importance as the change in the predictive distribution had the new observation $x_{i,t}$ not been seen. This is approximated by integrating over plausible counterfactuals, sampled from a distribution conditioned on individual history. By explicitly modeling the temporal behavior of the signals, we are able to determine the relative feature importance over time and find the most influential time point for every feature. Our method is model-agnostic, and can be applied to any complex model of any time series setting. We compare the generated feature importance to existing perturbation (Suresh et al., 2017) and gradient-based methods, attention mechanism (Bahdanau et al., 2014; Vaswani et al., 2017; Song et al., 2018), and other explanation baselines (Ribeiro et al., 2016). We show that our approach generates more precise explanations in simulated and real word settings and is the only approach that can identify critical time point for every feature in a time series.

2. Related Work
Various approaches have been proposed for explaining and understanding the behavior of time series models. In parameter visualization, recurrent model behavior is explained...
via visualization of latent activations of deep neural networks (Strobelt et al., 2018; Siddiqui et al., 2019; Ming et al., 2017). This approach is very helpful for experts trying to understand or debug a model, but it is too refined to be useful to the end users like clinicians, due to the complexity of network.

*Attention* (Bahdanau et al., 2014; Vaswani et al., 2017) can also be used to gain insight into time series model behavior. Attention models are suitable for sequential data and boost performance by learning to reliably learn from long range dependencies (Song et al., 2018; Kaji et al., 2019; Xu et al., 2018; Choi et al., 2016). These parameters in these models, called attention weights can be used to explain the model behavior over time. However, because of the complex mappings to latent space in recurrent models, attention weights cannot be directly attributed to individual observations of the time series (Guo et al., 2018). To obtain individual level feature importance, Choi et al. (2016) propose to augment the attention mechanism using separate sets of parameters to obtain importance scores over time and features separately. However, this does not allow to obtain the importance of each feature over time. Additionally, there are concerns regarding using attention weights as explanation because of consistency issues that have been observed (Jain & Wallace, 2019; Serrano & Smith, 2019).

Attribution methods explain models by evaluating the importance of each feature on the output. Attributions can be assigned using gradient-based methods to assess the sensitivity of the output to small changes in the input features (Bach et al., 2015; Yang et al., 2018; Hardt et al., 2019). These methods have to be carefully designed for time series settings, since the vanishing gradients in recurrent structures compromise the quality of feature importance assignment (Ismail et al., 2019). Perturbation-based approaches are an alternative method for assigning attribution. These methods assign higher importance to a feature that changes the model output the most, had it been different. This is often approximated by replacing the feature with mean value or random uniform noise (Fong & Vedaldi, 2017). A criticism of such methods is that the noisy perturbations can be out-of-domain for specific individuals and can lead to explanations that are not reflective of systematic behavior of the model Chang et al. (2019). As a clinical example, replacing a heart rate measurement of an individual of a specific age group with the population mean, can result in an observation that is highly unlikely under that patient distribution. This can lead to assigning a false high importance to that instance.

Evaluating sample based feature importance remains largely unstudied for time series models. While more widely studied for image classification, (Bach et al., 2015; Fong & Vedaldi, 2017) these methods cannot be directly extended to time series models for obtaining precise importances over time. In the next section, we propose a counterfactual-based method that explicitly models temporal dynamics in order to find the importance of features of multivariate time series at each point in time.

### 3. Method: Instance-wise Feature Importance in Time (FIT)

In this section we describe our method for generating observation-level feature importance as an explanation for time series models. We define the most important observation as the one with the largest influence on the output. Hence we measure the importance of an observation \( x_{i,t} \) as the change in the output distribution, assuming \( x_{i,t} \) had not been observed. We approximate this by replacing the observation with a realistic counterfactual conditioned on the history.

#### 3.1. Notation

A sample of a multi-variate time-series data is in the form of \( X^{(n)} \in \mathbb{R}^{d \times T} \), where \( d \) is the number of features with \( T \) observations over time. Throughout the paper, the index \( n \) over samples has been dropped for notational clarity. An observation, \( x_{i,t} \), is the value of feature \( i \) at time \( t \). Feature set with subscript \( -i \) indicates all features from the set [\( d \)] excluding feature \( i \). \( X_t \in \mathbb{R}^d \) is the vector \([x_{1,t}, x_{2,t}, \ldots, x_{d,t}]\) and \( X_{0:t} \in \mathbb{R}^{d \times t} \) is the matrix \([x_0, x_1, \ldots, x_t]\). We are interested in explaining a black-box estimator \( f_\theta \) that generates a probabilistic output over the label \( y_t \) at every time step \( t \), using observations up to that time point, \( X_{0:t} \in \mathbb{R}^{d \times t} \). Additional details on the notation used for exposition work is summarized in the Appendix A.1.

#### 3.2. Defining Importance

At each time \( t \), the observation that carries the most information about the model prediction can be said to be most important. We formalize this idea of importance by saying that, under some divergence measure, an observation is important if the predictive distribution, not having seen, the true \( x_{i,t} \) deviates significantly from the distribution \( p(y_t|X_{0:t}) \). We evaluate this based on the counterfactual influence of \( x_{i,t} \) on the prediction of the model. To reflect an accurate explanation, the counterfactual \( \hat{x}_{i,t} \) should be sample-specific and needs to reflect the signal history. We therefore sample it from the conditional distribution \( p(x_{i,t}|X_{0:t-1}) \). Intuitively, conditioning on the past \( 0 : t − 1 \), reflects the state of a feature at time \( t \) if there had been no change in the underlying dynamics. We argue that in time series, sampling from the distribution conditioned on the history of the signal, not only ensures that counterfactuals are realistic under the sample’s distribution, but also enables to retain critical time impor-
Figure 1. FIT procedure: The counterfactual 𝑥̂ᵣ is sampled from the generated conditional distribution. The predictor 𝑓 generates the output distribution for both the full observations 𝑋₀:𝑇 and the counterfactual 𝑋₀:𝑇. The KL-divergence between the two distributions measures the importance score.

3.3. Generative Model for conditional 𝑝(𝑥ᵢ | 𝑋₀:𝑡−1)
As mentioned in the previous section, 𝑥̂ᵣ is sampled from the conditional distribution 𝑝(𝑥ᵢ | 𝑋₀:𝑡−1). We approximate this distribution using a recurrent latent variable generator model 𝐺, introduced in Chung et al. (2015). 𝑥ᵣ is sampled from the distribution generated by the random variable 𝑧₄−𝑡 ∈ ℜ₄, which is the latent representation of the history up to time 𝑡 − 1. This distribution is approximated by a multivariate Gaussian with full covariance matrix to model potential correlation between features.

Algorithm 1 FIT
Input: 𝑓₀: Trained Black-box predictor model, time series 𝑋₀:𝑇, where 𝑇 is the max time and 𝐿: Number of Monte-Carlo samples

1: Train 𝐺
2: for all 𝑡 ∈ [𝑇] and 𝑖 ∈ [𝑑] do
3: 𝑝(𝑦ᵣ | 𝑋₀:𝑡) = 𝑓₀(𝑋₀:𝑡)
4: 𝑝(𝑥ᵢ | 𝑋₀:𝑡−1) ∼ 𝐺(𝑋₀:𝑡−1)
5: for all 𝑙 ∈ [𝐿] do
6: Sample 𝑥̂ᵣ,𝑙 ∼ 𝑝(𝑥ᵢ,𝑙 | 𝑋₀:𝑡−1)
7: 𝑝(𝑦ᵣ(𝑙)) = 𝑓₀(𝑋₀:𝑡−1, 𝑥ᵢ,𝑙, 𝑥̂ᵣ,𝑙)
8: 𝑝(𝑦ᵣ) = 𝑒𝑖𝑙𝑛𝑝(𝑦ᵣ(𝑙))
9: 𝑆ᵢ,𝑡 = 𝐾𝐿(𝑝(𝑦ᵣ | 𝑋₀:𝑡)) || 𝑝(𝑦ᵣ))
10: Importance_Matrix(𝑖, 𝑡) = 𝑆ᵢ,𝑡
11: Return Importance_Matrix

Note that the specifics of the generative model architecture can be a design choice. The quality of explanations generated by FIT, rely on the quality of the counterfactuals that need to reflect the underlying latent dynamics of signals. We have chosen a recurrent generator since it allows us to model non-stationarity in the time series while handling varying length of observations. We also compare the performance of simpler conditional generators and show that despite the drop in performance, FIT still outperforms other baselines even with a simpler generative model. Implementation details for the generator as well as the analysis results are provided in Appendix A.2.

3.4. Feature Importance Assignment Algorithm
The proposed procedure is summarized in Algorithm 1. We assume that we are given a trained black-box model 𝑓₀, and the data it had been trained on (no need for the labels). We first train a generator 𝐺, using the training data, to learn the conditional distribution 𝑝(𝑥ᵢ | 𝑋₀:𝑡−1). At every time point, 𝑥̂ᵣ is sampled from the distribution generated by 𝐺 and marginalized over 𝑥ᵢ,𝑙, i.e. the rest of the observations at time 𝑡. For a multivariate Gaussian distribution, this is equivalent to replacing 𝑥ᵢ,𝑙 with 𝑥̂ᵣ, 𝑋₀:𝑡 and 𝑋₀:𝑡 are then passed to the black-box model to evaluate the KL-divergence between the outcome distributions.

3.5. Properties
Our proposed method has the following compelling properties in explaining the estimator 𝑓₀:

- **Time Importance (TI)** For every feature of the time series, importance is assessed at every time step. With FIT, the most eventful time instances can be obtained as:

\[
\arg \max_{t \in [T]} \{ S_{i, t} \forall i \in [d] \}
\]
We can thus rank time instances in order of importance. That is, time $t_1 \leq t_2$, if $\max_{i \in [d]} \{S_{i,t_1}\} \geq \max_{i \in [d]} \{S_{i,t_2}\}$.

This is an important property for generating actionable explanations. For instance in a clinical setting, knowing whether a feature like blood pressure is relevant is not sufficient to intervene. A clinician would like to know when and what has happened that the model believed that blood pressure is important.

**Feature Importance (FI)** At any time instance $t$, our method also assigns importance to every feature $x_{i,t}$. The magnitude of our importance function reflects relative importance. Comparing the importance values across features also gives the flexibility to report a subset of important features at each time point $t$.

**4. Evaluation**

We evaluate our feature importance assignment method (FIT) on 2 simulated datasets and a real-world clinical dataset. For simulated data, ground-truth feature importance over time is available. Thus we directly evaluate our method by measuring the AUROC and AUPRC scores for identifying the important feature instances over time. We then apply our method to more complex clinical data to evaluate the performance on a real-world task. We compare with multiple baselines, described below.

1. **Feature Occlusion (FO)**: Introduced by Suresh et al. (2017), this method is a perturbation-based method where importance is assigned based on the difference in model prediction when each feature $x_i$ is replaced with a random sample from the uniform distribution.

2. **Augmented feature occlusion (AFO)**: We augment the method introduced in Suresh et al. (2017) by replacing observations with samples from the bootstrapped distribution $p(x_i)$ over each feature $i$. This avoids generating out-of-distribution samples.

3. **Sensitivity Analysis (SA)**: This method evaluates the sensitivity of the output for every observation, by taking the derivative of $y_t$ with respect to $x_{i,t}$, at every time point.

4. **LIME (Ribeiro et al., 2016)**: One of the most common explainability methods to assign local importance to features. Although LIME isn’t designed to assign temporal importance, for this baseline, we use LIME at every time point for a fair comparison.

5. **Attention (Bahdanau et al., 2014)**: While attention was first introduced as a mechanism to improve machine translation performance, recent works use the weights in attention models as a means for interpreting the importance of observations over time.

**4.1. Simulated Datasets**

Evaluating the quality of explanations is challenging due to the lack of a gold standard/ground truth for the explanations. Additionally, explanations are reflective of model behavior, therefore such evaluations are tightly linked to the reliability of the model itself. We therefore evaluate the functionality and performance of our baselines in a controlled simulated environment where the ground truth for feature importance is known. Experiment results on 2 different simulations are presented below, followed by a comparison to attention mechanisms.

**4.1.1. Simulated Data I: Spike Data**

We simulate a time series data such that only one feature determines the outcome. Specifically, the outcome (label) changes to 1 as soon as a spike is observed in the relevant feature. We keep the task fairly simple for two main reasons: 1) to ensure that the black-box classifier can indeed learn the right relation between the important feature and the outcome, which allows us to focus on evaluating the quality of the importance assignment without worrying about the quality of the classifier. 2) to have a gold standard for the explanations since the exact event predictive of the outcome is known. We expect the explanations to assign importance to only the one relevant feature, at the exact time of spike, even in the presence of spikes in other non-relevant features.

**Data generation:** We generate $d = 3$ (independent) sequences of standard non-linear auto-regressive moving average (NARMA) time series of the form:

$$x(t+1) = 0.5x(t) + 0.5x(t) \sum_{l=0}^{t-1} x(t-l) + 1.5u(t-(l-1))u(t) + 0.5$$

for $t \in [80]$, where the order is 2 and $u \sim N(0, 0.01)$. We add linear trends to the features and introduce random spikes over time for every feature. We train an RNN-based black-box predictor with AUC=0.99, and choose feature 0 (green on the plots) to be the important feature that determines the output $y_t$. The full procedure is described in Appendix A.4.

**Experiment results:** Figure 2 demonstrates explanations from each of the compared approaches for an illustrative sample from the testset. Note that all baseline methods provide an importance for every sample at each time point. The true explanation is to highlight the green feature at the time of the first spike. Using this ground truth, we evaluate the AUROC and AUPRC of the generated explanations. Table 1 summarizes these results. From Figure 2, we see that FIT identifies the right explanation by assigning importance to the green feature at the exact time of spike. FO fails to recover the important observation, and assigns random importance values to all features. This is due to the variance of perturbations drawn from the uniform distribution. AFO improves over this, by sampling from the marginal distri-
Figure 2. Spike Data: Results from a sample from the dataset. Figure on the top shows the 3 time series features and the dashed line indicates $y_t$, which switches from zero to one, only when the first spike appears in the green feature ($0$) from a black-box prediction model. Each following row shows the importance assignment scores for our method (FIT) and the baselines. Each line in this subplot corresponds to the importance value for one of the features, indicated by the color, over time. FIT assigns high importance to the green feature at the exact time of first spike. FO fails to identify the green spike as the variance of its perturbations are too high to be sensitive to spikes. Detailed comparison is included Section 4.1.1 and Table 1.

Figure 3. State Data: The top plot shows the time series signals and the output risk of the black-box model. Shaded regions indicate different hidden sates of the Markov model. The 4 lower plots are the importance assignments for FIT and other baselines. FIT assigns high importance at the exact critical time points of state change. AFO and FO are only able to find the most important feature in every state, but not the important time. And sensitivity analysis only detects the importance of later observations.
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| Method | Spike Data AUROC (exp) | Spike Data AUPRC (exp) | State Data AUROC (exp) | State Data AUPRC (exp) |
|--------|------------------------|------------------------|------------------------|------------------------|
| FIT (Ours) | **0.9985 ± 0.0006** | **0.8641 ± 0.0389** | **0.9269 ± 0.0094** | **0.161 ± 0.025** |
| AFO | 0.9721 ± 0.0132 | 0.4406 ± 0.2819 | 0.7594 ± 0.0105 | 0.0357 ± 0.0025 |
| FO | 0.8913 ± 0.0013 | 0.3368 ± 0.162 | 0.7581 ± 0.012 | 0.0359 ± 0.0015 |
| SA | 0.6188 ± 0.0363 | 0.0372 ± 0.0036 | 0.716 ± 0.0044 | 0.0407 ± 0.0008 |
| LIME | 0.3403 ± 0.0072 | 0.001 ± 0.0 | 0.5659 ± 0.0141 | 0.0229 ± 0.004 |

Table 1. Quantitative evaluation for simulated data using ground-truth feature importance. The proposed method detects important features with higher average precision compared to all baseline methods for both datasets, suggesting we capture the spike in the green feature (relevant feature and time) spike data and state changes along with important features in State Data more precisely than baselines.

Experiment results: Figure 3 shows the assigned importance for different features of the time series sample. The top plot is the time series data and shaded regions indicate the hidden state of the Markov model. The following rows show feature importance evaluation results for each baseline. AFO and FO capture the important feature in every state. However neither method characterizes temporal dynamics of the signal. The top importance values from each method therefore do not correspond to the state changes, i.e. important time points. The Sensitivity Analysis baseline is biased toward later observations, and therefore misses earlier state changes. This is because RNN-based black-box predictors are less sensitive to long source dependencies due to vanishing saliency (Ismail et al., 2019). Only FIT assigns high relative importance to features at times which corresponding to state changes. Table 1 compares performance across our baselines, measured as AUROC and AUPRC scores indicating the number of correct explanations assigned by each method. FIT provides a considerable improvement over all baselines in this task. Note that the AUPRC values are small for all methods, which is due to vast imbalance in false positive importances for the baseline methods.

4.1.3. EXPLAINING ATTENTION MODEL

Attention Models (Bahdanau et al., 2014; Vaswani et al., 2017), that are primarily used for seq2seq tasks in NLP, have also shown success in prediction tasks using time se-

bution which is more representative of the signals. This explains why it can identify the spike, and assigns more precise importance to features, compared to FO. Even if AFO ignores temporal dynamics, for this task, the conditional distribution modeled by FIT is reasonably approximated by the marginal. However, the magnitude of feature importance is not meaningful, resulting in the lower average precision of AFO in Table 1. Note that importance value for all features become zero after the spike, since nothing can change the output after that. Sensitivity analysis is gradient-based and can only capture changes to the prediction reliably for infinitesimally small perturbations, and not temporal dynamics. This baseline is thus able to locate the important time of spike in the green feature, however, the actual magnitude of gradient based importance values doesn’t distinguish the relative importance of the different features over time. More examples are provided in the Appendix A.3.

4.1.2. SIMULATED DATA II: STATE DATA

The first simulation ensures correct functionality of the method but does not necessarily evaluate it under complex state dynamics that is common in real-word time-series data. In this simulation, we create a dataset with a more complex temporal dynamics.

Data generation: The dataset consists of multivariate time series signals with 3 features. We use a non–stationary Hidden Markov Model with 2 latent states, and a linear transition matrix to generate observations over time. Specifically, at each time step $t$, observations are sampled from the multivariate normal distribution determined by the latent state of the HMM at that time. The non-stationarity models the state transition probabilities as a function of time. The outcome $y$ is a Bernoulli random variable, which, in state 1, is only determined by feature 1, and in state 2, by feature 2. The ground truth explanation for output at time $T$ is the observation $x_{i,t}$ where $i$ is the important feature for the current state and $t$ indicates when feature $i$ became important (state change). A full explanation for outcome at $t = T$ should include the most important feature variable as well as the time point of importance.

| Method | Spike Data AUROC (exp) | Spike Data AUPRC (exp) |
|--------|------------------------|------------------------|
| FIT (Ours) | **0.9908 ± 0.0001** | **0.566 ± 0.0025** |
| Attention | 0.9162 ± 0.0096 | 0.0411 ± 0.0018 |
| AFO | 0.9099 ± 0.0033 | 0.1447 ± 0.0304 |
| FO | 0.7735 ± 0.0348 | 0.0613 ± 0.0274 |
| SA | 0.3756 ± 0.0114 | 0.0014 ± 0.0 |

Table 2. Spike Data: Compared to attention scores, FIT provides more precise time importance, along with feature importance.
we compare generated explanations of different methods to performance quantitatively on simulated data, we test our proposed method assigns time importance with much higher average precision than the attention weights. This is because the attention model assigns high weights to all observations that lead to the outcome, and fails to identify the most informative observation over time.

### 4.2. MIMIC Mortality Prediction Model

Explaining models based on feature and time importance is critical for clinical settings. Therefore, having verified performance quantitatively on simulated data, we test our methods on a more complex mortality prediction task for the Intensive Care Unit (ICU). The black-box model is an RNN-based mortality prediction model, trained on time series data from the MIMIC-III dataset. The data consists of de-identified EHRs for ∼ 40,000 ICU patients at the Beth Israel Deaconess Medical Center, Boston, MA and includes time series measurements such as vitals and lab results over patients’ ICU stay (Johnson et al., 2016). The RNN-based black-box model uses static patient information (age, gender, ethnicity), 8 vital measurements and 20 lab results to predict mortality in the next 48 hour. Further details on the model and data can be found in Appendix A.5.

Following the procedure in Algorithm 1, we train a conditional generator for the time series features (vitals and lab measures) to assign importance over time using FIT. Figure 4 shows a sample heatmap of the importance of each clinical measurement, at every hour during a patient’s ICU stay (assigned by our method). Similar heatmap results for other baselines are also provided in Appendix A.5. To compare results across different methods, we also look into the importance assignment of our baselines in Figure 5. The top plot shows the trajectory of multiple signals for this specific individual, and the dashed black line indicates the model prediction. The plots below visualize importance scores over time for the top most important signals.

As shown in Figure 5, AFO, FO and FIT pick almost the same signals as important features for this individual patient and the importance peaks around similar time. While sensitivity analysis identifies the critical time point, it fails to infer the correct relative importance for the features. Due to lack of ground truth for explanations, we use global importance as a proxy for evaluation. In future work, this evaluation can be done with the help of domain experts, i.e. ICU clinicians.

| Method   | AUROC (exp) | AUPRC (exp) |
|----------|-------------|-------------|
| FIT (Ours) | **0.9482 ± 0.0047** | **0.5407 ± 0.0112** |
| Attention | 0.6522 ± 0.0358 | 0.1827 ± 0.0156 |
| AFO      | 0.7786 ± 0.0287 | 0.1896 ± 0.0096 |
| FO       | 0.7608 ± 0.0311 | 0.1658 ± 0.0146 |
| SA       | 0.8061 ± 0.0169 | 0.2109 ± 0.0188 |
| LIME     | 0.4762 ± 0.0006 | 0.0504 ± 0.0009 |

Table 3. State Data: Comparison of attention scores, FIT provides the exact time instances of state changes whereas Attention focuses on all observations in a given state that predict the outcome.

| Method          | AUROC -model w/o top 10 | AUROC -model w/ top 3 only |
|-----------------|--------------------------|---------------------------|
| FIT             | 0.7787 ± 0.0008          | 0.7206 ± 0.0012           |
| AFO             | 0.7796 ± 0.0004          | 0.7217 ± 0.0009           |
| FO              | 0.7855 ± 0.0012          | 0.7203 ± 0.0007           |
| SA              | 0.7816 ± 0.0028          | 0.6939 ± 0.0009           |
| LIME            | 0.7808 ± 0.0024          | 0.6797 ± 0.0003           |

Table 4. Real Data - Global Importance. Prediction model deteriorates the most when top 10 features according to FIT are removed suggesting it reliably captures global relevance and provides competitive performance, just after AFO when trained only on top 3 features according to FIT.

### 4.2.1. Evaluation Using Global Importance

Another way to quantitatively evaluate the proposed method on real data, is to assess how well the method performs at
selecting globally important features. We evaluate global importance by studying i) how much the prediction model performance deteriorate if the top 10 most relevant features according to each method are removed (lower is better) and ii) how well the prediction model performs if trained using only the top 3 relevant features determined by the method (higher is better). The results in Table 4 demonstrate that the proposed method is competitive at assigning population level importance.

4.3. Sanity Check Test for Explanations

We additionally evaluate the quality of the proposed FIT method using the parameter randomization test proposed as ‘Sanity Checks’ in (Adebayo et al., 2018). We use cascading randomization by gradually randomizing model weights and evaluating the rank correlation of explanations generated on the randomized model to the explanation of the original model. A method is reliable if its explanations of the randomized model and original model are uncorrelated, with increased randomization further reducing the correlation between explanations. Figure 6 demonstrates that our method passes this check as the explanations from the randomized models have little correlation with the original explanations.

5. Discussion

In this work, we propose a general approach for assigning importance to observations in a multivariate time series. We evaluate the importance of each observation by its counter-
factual effect on the predictive distribution. We compare the proposed definition and algorithm to several existing approaches and show that our method is better at localizing important observations over time. Our results show that existing perturbation based methods are good for ranking features at every time step, but are not able to find the time instances with highest importance. Gradient based methods, like sensitivity analysis, rank features appropriately at later time instances but fail to assign importance to earlier observations of long temporal sequences. Even in attention models, our method recovers time importance more reliably, as demonstrated by the results in Table 2. Our method provides explanation at observation level (every feature at every time step) efficiently (as shown by the run time analysis in Appendix A.6). FIT is model agnostic and can be used for arbitrarily complex models and different time series data.

5.1. Software and Data
Software used: Python 3.7.3, Pytorch 1.0.1.post2
GPU Info: Quadro 400
CPU Info: Intel(R) Xeon(R) CPU E5-1620 v4 @ 3.50GHz

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A. Appendix

A.1. Notation

Summary of notations used throughout the paper

| Notation | Description |
|----------|-------------|
| $[K]$ for integer $K$ | Set of indices $[K] = \{1, 2, \ldots, K\}$. |
| $i, t$ | Index for feature $i$ in $[d]$, time step $t$. |
| $i \neq t$ | Set $[d] \setminus i$. |
| Data | |
| $x_{i,t}$ | Observation $i$ at time $t$. |
| $x_d \in \mathbb{R}^d$ | Vector $[x_{1,t}, x_{2,t}, \ldots, x_{d,t}]$. |
| $X_{0:t} \in \mathbb{R}^{d \times t}$ | Matrix $[x_0, x_1, \ldots, x_t]$. |
| $p(y_i | X_{0:t}) \triangleq f(X_{0:t})$ | Outcome of the model $f$, at time $t$. |

Table 5. Notation used in the paper.

A.2. Generative Model for Conditional Distribution

A.2.1. RECURRENT GENERATIVE MODEL

We approximate the conditional distribution using a recurrent latent variable generator model $G_t$ as introduced in (Chung et al., 2015). The latent variable $Z_t$ is the representation of the history of the time series up to time $t$, modeled with a multivariate Gaussian with a diagonal covariance. The conditional distribution of the counterfactual is modeled as a multivariate Gaussian with full covariance, using the latent sample $Z_t$.

![Graphical model representation of the conditional generator. $Z_t$ is the latent representation of the signal history up to time $t$. The counterfactual $\hat{x}_{t+1}$ will be sampled from the distribution generated by the latent representation.](image)

Other generator models can also be used with our method. We evaluate the effect of the choice of generator to the quality of the explanations. We compare performance to another recurrent generative model, with shorter history (only 5 steps in the past), as well as a simple generator that samples the counterfactual from the distribution conditioned only on the last observation (Namely Carry forward). Results are presented in Table 6. Simpler generators have a slightly lower performance in exchange for simplicity and faster run-time. In future work, it is interesting to characterize the effect of bias in generative models on the quality of explanations.

In order to obtain accurate explanations, the generative model should model the conditional distribution approximated by the recurrent neural network based generative model.

![Feature importance performance with other generative models.](image)

Table 6. Feature importance performance with other generative models.

| Features | KS test statistic | p-value |
|----------|------------------|---------|
| feature 0 | 0.0018           | 1.0     |
| feature 1 | 0.0021           | 1.0     |
| feature 2 | 0.0022           | 0.9999  |

Table 7. State data: KS Test statistic and p-value for evaluating the quality of the conditional distribution approximated by the recurrent neural network based generative model.

A.3. Simulated Data I

A.3.1. DATA GENERATION

To simulate these data, we generate $d = 3$ (independent) sequences as a standard non–linear auto-regressive moving average (NARMA) time series. Note also that we add linear trends to features 1 and 2 of the form:

$$x(t + 1) = 0.5x(t) + 0.5x(t) \sum_{l=0}^{t-1} x(t - l) + 1.5u(t - (l - 1))u(t) + 0.5 + \alpha_d t$$

for $t \in [80]$, $\alpha > 0$ (0.065 for feature 2 and 0.003 for feature 1), and where the order $l = 2$, $u \sim$ Normal(0, 0.03). We additionally add linear trends to features. We add spikes to each sample (uniformly at random over time) and for each feature $d$ following the procedure below:

$$y_d \sim \text{Bernoulli}(0.5);$$

$$\eta_d = \begin{cases} 
\text{Poisson}(\lambda = 2) & \text{if } 1(y_d = 1) \\
0 & \text{otherwise}
\end{cases}$$

$$g_d \sim \text{Sample}([T], \eta_d); x_{d,t} = x_{d,t} + \kappa \forall t \in g_d$$

We evaluate the quality of the generative model using 2-sample tests such as the Kolmogorov–Smirnov test. While we do this per feature, other two sample tests for multivariate data may also be used (Gretton et al., 2012; Lopez-Paz & Oquab, 2016). Table 7 shows the test statistic and $p$-values for the recurrent generative model used in our the State data experiment (compared with samples from the true conditional State data distribution). If the distributions are identical, we expect to see a high $p$-value or a much lower value of the KS-test statistic indicating that the null hypothesis (the two distributions are the same) cannot be rejected.
where $\kappa > 0$ indicates the additive spike. The label $y_t = 1 \forall t > t_1$, where $t_1 = \min g_d$, i.e. the label changes to 1 when a spike is encountered in the first feature and is 0 otherwise. We sample our time series using the python TimeSynth\(^1\) package.

A.3.2. IMPLEMENTATION DETAILS

Our generator $G_i$ is a single layer RNN (GRU) with encoding size 50. The total number of samples used is 10000 (80\%-20\% split) and we use Adam optimizer for training on 250 epochs.

A.3.3. ADDITIONAL SAMPLES

Additional sample results for the Spike experiment are provided in Figures 8 for an RNN-based prediction model. We additionally plot the attention weights of an attention-based prediction model with similar structure to the RNN-based black-box model.

A.4. Simulated Data II

A.4.1. DATA GENERATION:

In this dataset, the random states of the time series are generated using a two state HMM with $\pi = [0.5, 0.5]$ and transition probability $T$:

$$T = \begin{bmatrix} 0.1 & 0.9 \\ 0.1 & 0.9 \end{bmatrix}$$

The time series data points are sampled from the distribution emitted by the HMM. The emission probability in each state is a multivariate Gaussian: $N(\mu_1, \Sigma_1)$ and $N(\mu_2, \Sigma_2)$ where $\mu_1 = [1.2, 1.5, 0.8]$ and $\mu_2 = [-1.2, -0.8, -1.5]$. Marginal variance for all features in each state is $0.8$ with only features 1 and 2 being correlated ($\Sigma_{12} = \Sigma_{21} = 0.01$) in state 1 and only 0 and 2 on state 2 ($\Sigma_{02} = \Sigma_{20} = 0.01$).

The output $y_t$ at every step is assigned using the logit in 5. Depending on the hidden state at time $t$, only one of the features contribute to the output and is deemed influential to the output. In state 1, the label $y$ only depends on feature 1 and in state 2, label depends only on feature 2.

$$p_t = \begin{cases} \frac{1}{1 + e^{-s_t}} & s_t = 0 \\ \frac{1}{1 + e^{-s_t}} & s_t = 1 \end{cases}$$

$$y_t \sim Bernoulli(p_t)$$

A.4.2. IMPLEMENTATION DETAILS

Our generator $G_i$ is trained using a one layer, forward RNN (GRU) with encoding size 10. The generator is trained using the Adam optimizer over 800 time series sample of length 200, for 300 epochs.

A.4.3. ADDITIONAL SAMPLES

Additional examples for state data experiment are provided in Figure 9.

A.5. MIMIC-III Mortality Experiment

A.5.1. FEATURE SELECTION AND DATA PROCESSING:

For this experiment, we select adult ICU admission data from the MIMIC-III dataset. We use static patients’ static, vital measurements and lab result for the analysis. The task is to predict 48 hour mortality based on 48 hours of clinical data, therefore we remove samples with less than 48 hours of data. Table 8 presents a full list of clinical measurements used in this experiment.

The predictor model takes in new measurements every hour, and updates the mortality risk. We quantize the time series data to hour blocks by averaging existing measurements within each hour block. We use 2 approaches for imputing missing values: 1) Mean imputation for vital signals using the sklearn SimpleImputer\(^2\), 2) forward imputation for lab results, where we keep the value of the last lab measurement until a new value is evaluated. We also removed patients who had all 48 quantized measurements missing for a specific feature. Overall, 22,988 ICU admissions were extracted and training process was on a 65\%,15\%,20\% train, validation, test set respectively.

A.5.2. IMPLEMENTATION DETAILS:

The mortality predictor model is a recurrent network with GRU cells. All features are scaled to 0 mean, unit variance and the target is a probability score ranging $[0, 1]$. The model achieves $0.7939 \pm 0.007$ AUC on test set classification task. Detailed specification of the model are presented in Table 9. The conditional generator is a recurrent network with specifications shown in 10.

A.5.3. ADDITIONAL SAMPLES:

Additional example results for MIMIC-III are provided in Figure 10.

A.5.4. EXPLANATION EVALUATION USING CLINICAL ANNOTATIONS

As a proxy for evaluation, we use the intervention information present in patient records to evaluate clinical applicability across baselines. Clinicians intervene with a medication

\(^{1}\)https://github.com/TimeSynth/TimeSynth
\(^{2}\)https://scikit-learn.org/stable/modules/generated/sklearn.impute.SimpleImputer.html
Figure 8. Additional examples from the state data experiment
Figure 9. Additional examples from the state data experiment
Individualized Feature Importance for Time-series Models

![Graphs showing feature importance over time for various features like BICARBONATE, PHOSPHATE, and INR.](image)

Figure 10. Additional examples from the MIMIC-III experiment
Individualized Feature Importance for Time-series Models

Table 8. List of clinical features for the risk predictor model

| Setting                  | Value                                                                                                                                 |
|--------------------------|---------------------------------------------------------------------------------------------------------------------------------------|
| epochs                   | 80                                                                                                                                      |
| Model                    | GRU                                                                                                                                    |
| Encoding size ($m$)      | 150                                                                                                                                     |
| Loss                     | MSE                                                                                                                                     |
| Regressor Activation     | Sigmoid                                                                                                                               |
| Dropout                  | True                                                                                                                                    |
| Gradient Algorithm       | Adam ($\alpha = 0.001, \beta_1 = 0.9, \beta_2 = 0.999, \text{weight decay} = 0$)                                             |

Table 9. Mortality risk predictor model features.

| Setting                  | Value                                                                                                                                 |
|--------------------------|---------------------------------------------------------------------------------------------------------------------------------------|
| epochs                   | 150                                                                                                                                      |
| RNN cell                 | GRU                                                                                                                                     |
| batch normalization      | True                                                                                                                                    |
| encoding size            | 80                                                                                                                                      |
| Regressor encoding size  | 300                                                                                                                                     |
| Loss                     | MSE                                                                                                                                     |
| Gradient Algorithm       | Adam ($\alpha = 0.0001, \beta_1 = 0.9, \beta_2 = 0.999, \text{weight decay} = 0$)                                             |

Table 10. Training Settings for Feature Generators for MIMIC-III Data

**Figure 11.** Top four features assigned to be important for each intervention across compared methods.

A.6. Run-time analysis

| Method | Simulation data (sec) | MIMIC data (sec) |
|--------|-----------------------|------------------|
| FIT    | 2.5                   | 0.97             |
| AFO    | 1.64                  | 0.59             |
| FO     | 1.05                  | 0.35             |
| LIME   | 0.76                  | 0.33             |
| SA     | 0.189                 | 0.078            |

Table 11. Run-time results for simulated data and MIMIC experiment.

In this section we compare the run-time across multiple baselines methods on a machine with Quadro 400 GPU and Intel(R) Xeon(R) CPU E5-1620 v4 @ 3.50GHz CPU. The results are reported in Table 11, and represent the time required for evaluating importance value of a feature over $T$, in seconds.

Note that for all methods, runtime is directly correlated with the length of the time series. What slows down performance on FIT, is the amount of history that it uses for generating the conditional distribution. In this experiment, we used the entire signal history for every inference, however, by reducing the size of the history window, we can reduce the run time, without notable sacrifice to performance. We show that by reducing the memory window of the generator to 5 steps, the inference run time reduces to 2.09 sec.