AnomalyKiTS: Anomaly Detection Toolkit for Time Series

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Abstract
This demo paper presents a design and implementation of a system AnomalyKiTS for detecting anomalies from time series data for the purpose of offering a broad range of algorithms to the end user, with special focus on unsupervised/semi-supervised learning. Given an input time series, AnomalyKiTS provides four categories of model building capabilities followed by an enrichment module that helps to label anomaly. AnomalyKiTS also supports a wide range of execution engines to meet the diverse need of anomaly workloads such as Serveless for CPU intensive work, GPU for deep-learning model training, etc.

Introduction
With wider adoption of Industry 4.0, many industrial applications are harvesting data from ongoing processes in real time. The collected data are of increasingly wide range of formats such as time series, images, alarms, quality inspection reports, etc. Among all these diverse data modalities, time series is the most common data format across multiple applications and has recently gained significant attention. For example, our recent work in the time series domain includes AutoAI-TS (Shah et al. 2021), Smart-ML (Patel et al. 2020a), TransformerML (Zerveas et al. 2021), FLOps (Patel et al. 2020b), etc.

Broadly, two types of time series data analysis toolkits are developed in the literature: General purpose toolkits such as sktime (Löning et al. 2019), pyFTS (Silva et al. 2018), tseries (Hyndman and Yang 2018. v0.1.0), tslearn (Tavenard et al. 2020), GluonTS (Alexandrov et al. 2020) etc, and purpose-built toolkits such as Anomaly Detection toolkits (Zhao, Nasrullah, and Li 2019; Ying et al. 2020; Ren et al. 2019; Zhang, Nie, and Yuan 2020; Buda, Caglayan, and Assem 2018; Gao et al. 2020; Geiger et al. 2020; Lee, Lin, and Gran 2020; Bhatnagar et al. 2021), etc. The former one provides a range of algorithms to the end user for quick exploration; on the other hand, the latter one is tailored to support a specific usecase and is more rigid in the customization. We noticed a recent surge in unsupervised learning based anomaly toolkits. This is due to the fact that obtaining a label for supervised learning in an automated and reliable manner is a challenging task for time series data.

Although both types of system development aim to enable easy access to build anomaly solutions centered around time series, current systems overload the user with a large variety of options and APIs. Some form of standardization, formal definition and automation of the anomaly task is required. Scikit-learn library (Buitinck, Louppe, and etl 2013) has been popular among data scientists, but it is limited to mostly tabular data. The sktime (tslearn) library extended definition to support time series data but mainly concentrated on forecasting (classification) functionality. PyOD is the popular outlier detection toolkit but lacks support for time series data. Moreover, the data size and the nature of anomaly varies from application to application, and the current off-the-shelf toolkits do not cover all the usecases such as Semi-supervised anomaly, Prediction Based unsupervised anomaly, etc. In this demo paper, we present a design and implementation of a system that enables data scientists and AI practitioners to get a unified access to various anomaly detection machinery for time series data.

AnomalyKiTS : System Overview

Figure 1 gives an overview of AnomalyKiTS’s layered architecture. AnomalyKiTS is based on Sklearn compliant standardized architecture, components and output schema.

Figure 1: Layered architecture of AnomalyKiTS
Anomaly Operators. The bottom-most layer consists of basic machine learning primitives such as Estimators, Transformers, Outlier Detectors, Data Stationarizers, etc. These components tend to perform one specific task/function and are referred to as Operators. At present, we have implemented 30+ Operators for anomaly related tasks along with the components that are already available in other libraries.

Anomaly Pipelines. The second layer implements advanced machine learning primitives in the form of an anomaly pipeline that logically connects different components from the lower layer. We introduced 4 types of anomaly pipelines:
- DeepAD
- RelationshipAD
- ReconstructAD
- WindowAD

These four pipelines cover a wide range of anomaly detection approaches such as: DeepAD uses an ensemble of time series forecasting models for anomaly detection (Buda, Caglayan, and Assem 2018), whereas RelationshipAD is based on the pair-wise relationship between variables for anomaly detection (Zong et al. 2018; Liu et al. 2018). Apart from generating the anomaly score in a unique way, each of the pipelines provides an additional capability in the form of “anomaly thresholding” to generate the anomaly labels (+1 for normal sample and -1 for anomalous) and if possible the predicted contribution of an individual variable. The pipeline supports two types of anomaly labeling methods: Static and Dynamic.

Anomaly Workflow. The left side of the third layer is a core data science workflow module and is inspired by the fact that, the data scientist would be interested in exploring multiple pipelines and picking the one that meets their need. To simplify the multiple pipelines specification, we adopted a Directed Acyclic Graph (DAG) based workflow construction as discussed in detail (Shrivastava et al. 2019; Patel et al. 2020a). Along with DAG, user can also configure the parameters for each forecasting pipeline to conduct hyper-parameter tuning.

Execution Engines. The right side of the third layer is an execution engine for scalable workflow exploration. This layer is an important module to meet the need of exploring multiple pipelines and/or single pipeline with a large dataset in an efficient and scalable way. Compared to other libraries, our system provides a more uniform access to multiple execution platforms such as Watson Machine Learning for GPU based training, Spark and Serverless (Ray, Cloud Function, Code Engine) for CPU intensive task level parallelism, etc.

Anomaly Usecases. The top most layer is an application layer that offers various pre-built industrial templates to build reusable applications. In the case of un-supervised exploration, our system provides several ranking methods such as EM Score and AL Score (Goix 2016) that do not require explicit label information. In the case of semi-supervised exploration, the user provides a small amount of labeled data for obtaining the rank of each pipeline in the Workflow.

**AnomalyKiTS : Benchmark and Deployment**

AnomalyKiTS is tested for various datasets ranging from synthetically generated time series data (e.g., Argots) to client engagement, and public sources (Geiger et al. 2020; Wu and Keogh 2021). In the following Figure 2, we provided box plot of more that 10,000 experiments on various Static anomaly thresholds. Briefly, we train various WindowAD based anomaly detection algorithms, and then apply different scoring method to obtain the anomaly label. The generated anomaly label is compared with available ground truth. We used “recall” of an algorithm as a ranking criteria. X axis is average rank and Y-axis is various scoring methods with different parameter settings. In this case, a parameter-free “ostu” method turns out to be a winner.

![Figure 2: Benchmark : 80+ public datasets](image)

**Service Deployment.** AnomalyKiTS is deployed on IBM API Hub. Currently it supports two types of requests:
- **Batch mode.** scan the entire time series and detect the anomaly from anywhere
- **Train-Test mode.** use the historical data as a training and then detect anomaly in the most recent data

![Figure 3: Anomaly Service Testing on Code Engine](image)

For each incoming request, Anomaly services obtain new training resources (i.e., CPU/GPU) using Serverless Code Engine or Watson Machine Learning. Figure 3 shows the promptness of the service to handle homogeneous workload of 43 incoming requests using IBM Code Engine. Each request was allocated 4 CPU with 16 GB RAM and the size of the data varies up to 10k record and 5 features.

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1https://developer.ibm.com/apis/catalog/ai4industry--anomaly-detection-product/Introduction
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