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OnlineBootKNN: An Unsupervised Framework for Detecting Anomalies in Spectral Data Streams

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Monitoring the elemental composition of materials in order to detect abnormal conditions in real-time is essential for applications like manufacturing quality control, environmental monitoring, and space exploration. This is achieved using sensors that analyze the interaction of a material with electromagnetic radiation, producing spectral data streams or a sequence of instances where each represents an ordered set of wavelengths with an associated intensity. While many unsupervised anomaly detection methods exist for tabular streaming data, their applicability to spectral streams remains underexplored. To address this gap, we consider our spectra in a multivariate stream setting and benchmark the performance of state-of-the-art tabular anomaly detection methods on this data. Furthermore, we introduce OnlineBootKNN, a novel unsupervised framework that combines k-nearest neighbors with online bootstrapping and a z-score test to detect anomalies in real-time. We demonstrate the high performance and robustness of our method, as well as the efficacy of the autoencoder-based method, KitNet, on newly simulated real-world spectral datasets. In addition, we compare their efficiency against the other tested techniques. Finally, we highlight the inherent interpretability of OnlineBootKNN, which is crucial for identifying the specific wavelengths, and thus elements, responsible for a detected anomaly.

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