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nonconform: Conformal Anomaly Detection (Python)

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Summary

The ability to quantify uncertainty is a fundamental requirement for AI systems in safety-critical and costly-to-error domains, as reliable decision-making strongly depends on it. The Python package `nonconform` offers statistically principled uncertainty quantification for semi-supervised anomaly detection based on one-class classification (Petsche & Gluck, 1994). The package implements methods from conformal anomaly detection (Bates et al., 2023; Jin & Candès, 2023; Laxhammar & Falkman, 2010), grounded in the principles of conformal inference (Lei & Wasserman, 2013; Papadopoulos et al., 2002; Vovk et al., 2005).

The `nonconform` package calibrates anomaly detection models to produce statistically valid p-values from raw anomaly scores. The calibration process uses a hold-out set $\mathcal{D}_{\text{calib}}$ of size n containing normal instances, where the model has been trained on a separate set of normal data. For a new observation X_{n+1} with anomaly score $\hat{s}(X_{n+1})$, this is achieved by comparing it to the empirical distribution of calibration scores $\hat{s}(X_i)$ for $i \in \mathcal{D}_{\text{calib}}$. The conformal p-value $\hat{u}(X_{n+1})$ is then defined as the normalized rank of $\hat{s}(X_{n+1})$ among the calibration scores (Liang et al., 2024):

$$\hat{u}(X_{n+1}) = \frac{|\{i \in \mathcal{D}_{\text{calib}} : \hat{s}(X_i) \leq \hat{s}(X_{n+1})\}|}{n}.$$

By framing anomaly detection as a sequence of statistical hypothesis tests, these p-values enable systematic control of the False Discovery Rate (FDR) (Bates et al., 2023; Benjamini & Hochberg, 1995) at a pre-defined significance level by respective statistical procedures. The library integrates seamlessly with the widely used `pyod` library (Chen et al., 2024; Zhao et al., 2019), facilitating the application of conformal techniques across a broad range of anomaly detection models.

Statement of Need

A central challenge in anomaly detection lies in setting an appropriate detection threshold, as it directly determines the false positive rate. In high-stakes domains such as fraud detection, medical diagnostics, and industrial quality control, controlling false positives is critical: excessive false alarms can cause *alert fatigue* and ultimately render a system impractical. The `nonconform` package addresses this issue by replacing raw anomaly scores with p-values, thereby enabling formal FDR control. As a result, the conformal methods become effectively *threshold-free*, since decision thresholds are determined by the underlying statistical procedures.

$$FDR = \frac{\text{Efforts Wasted on False Alarms}}{\text{Total Efforts}}$$

(Benjamini et al., 2009)

Moreover, conformal methods are *non-parametric* and *model-agnostic*, and thus apply to any model that produces consistent anomaly scores on arbitrarily distributed data. A key requirement of these methods is the statistical assumption of exchangeability between calibration and test data, which ensures the validity of conformal p-values. Exchangeability requires only that the joint distribution of data is invariant under permutations, making it considerably more general (and thus less restrictive) than the independent and identically distributed (*i.i.d.*) assumption commonly imposed in classical machine learning.

To operationalize this assumption in practice, the `nonconform` package provides several strategies for constructing calibration sets from training data, including approaches tailored to low-data regimes (Hennhofer & Preisach, 2024), that do not rely on a dedicated hold-out set. Based on obtained calibration sets, the package derives either standard conformal p-values or weighted conformal p-values (Jin & Candès, 2023), which are particularly useful under covariate shift when exchangeability is only approximate. By offering these tools, `nonconform` enables researchers and practitioners to build anomaly detectors whose outputs are statistically controlled to maintain the FDR at a chosen nominal level.

Overall, the reliance on exchangeability makes these methods well suited for cross-sectional data, but less appropriate for time-series applications where temporal ordering carries essential information.

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