

## Outlier Detection in Medical Diagnostic Data: A Comparative Study on the Wisconsin Breast Cancer Dataset

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#### Outline



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- Labeled medical records are scarce and expensive to obtain; unsupervised outlier detection can flag risky cases and assist medical professionals.
- Early flagging of malignant outliers can speed up treatment, improving patient outcomes.
- In high-dimensional data the curse of dimensionality makes distance unreliable, so we need structure-based ways to spot outliers.

## Survey Scope and Method Choice



- We study unsupervised and semi-supervised outlier detection for structured, high-dimensional medical data.
- We compare three established methods—Isolation Forest, Local Outlier Factor, and One-Class SVM—that stand for diverse approaches.
- Isolation Forest splits data at random, LOF calculates local density, and One-Class SVM draws a boundary in kernel space.
- Each method lives in standard libraries and appears in real studies, so the set gives a clear, reproducible benchmark.



- Dataset: Breast Cancer Wisconsin (Diagnostic) 569 samples, 30 numeric features drawn from fine-needle aspirate images.
- Each record carries a label: benign = B or malignant = M.
- Data are complete and clean; we apply z-score standardisation and a stratified train-test split using scikit-learn.
- Training uses benign cases to reflect semi-supervised practice; evaluation covers both classes.



- Ensemble-based partitioning exploits random partitioning of the feature space.
- Builds many random trees and measures how fast each point gets isolated.
- Anomalies need fewer splits, so they sit near the tree roots.
- Runs in  $O(n \log n)$  time and keeps memory use low. Works well in high-dimensional data (Liu et al. (2008))
- Few parameters: number of trees and sub-sample size.

## Local Outlier Factor (LOF)



- Density-based locality focuses on deviations in neighbourhood density.
- Compares the local density of each point to that of its neighbours.
- A point with much lower density than its k neighbours scores as an outlier.
- Handles clusters of different shapes because it stays local. (Breunig et al. (2000))
- Needs *k* and a distance metric; sensitive to both.



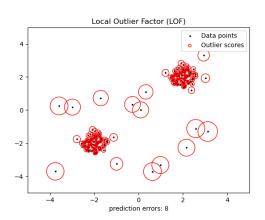


Figure: Taken from scikit-learn documentation.



- Kernel boundary learning treats outlier detection as a one-class classification task.
- Learns a boundary that encloses normal data in high-dimensional kernel space.
- Points outside the boundary count as anomalies.
- Works with any kernel; we use the Radial Basis Function.
- Training is  $\mathcal{O}(n^2)$  in practice, so scaling is harder.

## Implementation Details (I)



- **Environment**: Python 3.11 with scikit-learn 1.4 Pedregosa et al. (2011).
- Dataset load: load\_breast\_cancer() from sklearn.datasets (Dua and Graff, 2019).
- Pre-processing
  - Standardise features using StandardScaler.
  - Stratified 80 / 20 train-test split.
- Workflow: separate scripts for data, models, and plots; each step can run end-to-end from a single shell command.
- Reproducibility: fixed random\_state = 61; repository on GitHub.



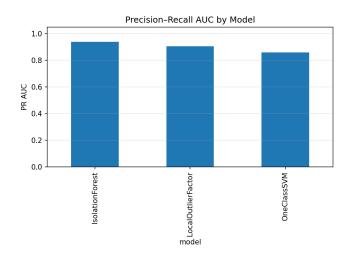
#### Training protocol

- Fit each model on benign training data.
- Predict anomaly scores on the held-out set (benign + malignant).

#### **Evaluation metrics**

- ROC AUC separates classes across thresholds .
- PR AUC focuses on the minority class, more informative under imbalance (Saito and Rehmsmeier (2015)).



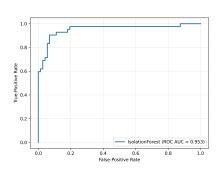


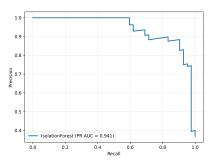


- Isolation Forest ranks first PR AUC 0.94, ROC AUC 0.95. best performer.
- Local Outlier Factor follows PR AUC 0.91, ROC AUC 0.93. Density checks work, yet high dimensionality blurs neighbourhoods and costs 4 pp in precision-recall.
- One-Class SVM trails PR AUC 0.86, ROC AUC 0.92.
   The kernel boundary fits the overall data well, but it lets more malignant samples slip past the boundary.
- All three beat random guessing by a wide margin.

## Isolation Forest – ROC and PR Curves

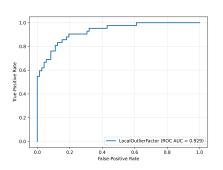


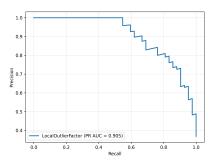




### Local Outlier Factor – ROC and PR Curves

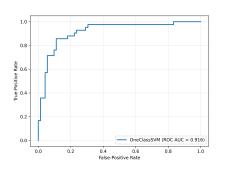


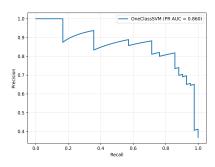




#### One-Class SVM - ROC and PR Curves









- Dimensionality reduction the current pipeline keeps all 30 features; techniques such as PCA could cut noise and reveal stronger patterns (Aggarwal and Yu, 2001).
- Hyperparameter tuning every model still runs on default settings; a grid search could lift accuracy and stability, especially for LOF and One-Class SVM.
- Interpretability clinicians need clear reasons for each alert; today's scores explain little, so methods that map anomalies back to patient features are still critical. (Zimek et al., 2012).



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- Code: full pipeline and figures
- Run: python main.py
- Reproduce: same metrics, same plots



- Aggarwal, C. C., & Yu, P. S. (2001). Outlier detection for high dimensional data. ACM SIGMOD Record, Volume 30, Issue 2, 37–46.
- Aktepe, S. C. (2022). Middle east technical university unofficial presentation template.
- Breunig, M. M., Kriegel, H.-P., Ng, R. T., & Sander, J. (2000).Lof: Identifying density-based local outliers. *Proceedings of the 2000 ACM SIGMOD international conference on Management of data*, 93–104.
- Dua, D., & Graff, C. (2019). Uci machine learning repository: Breast cancer wisconsin (diagnostic) data set [Accessed: 2025-05-11]. https://archive.ics.uci.edu/ml/datasets/Breast+Cancer+Wisconsin+(Diagnostic)



- Liu, F. T., Ting, K. M., & Zhou, Z.-H. (2008). Isolation forest. 2008

  Eighth IEEE International Conference on Data Mining, 413–422.
- Pedregosa, F., Varoquaux, G., Gramfort, A., Michel, V., Thirion, B.,
  Grisel, O., Blondel, M., Prettenhofer, P., Weiss, R., Dubourg,
  V., et al. (2011).Scikit-learn: Machine learning in python. *Journal of Machine Learning Research*, 12.
- Saito, T., & Rehmsmeier, M. (2015). The precision-recall plot is more informative than the roc plot when evaluating binary classifiers on imbalanced datasets. *PloS One*, *10*(3), e0118432.
- Zimek, A., Schubert, E., & Kriegel, H.-P. (2012). A survey on unsupervised outlier detection in high-dimensional numerical data. *Statistical Analysis and Data Mining: The ASA Data Science Journal*, *5*(5), 363–387.



# Thank You for your attention.

Do you have any question?