CatBoost, XGBoost, and LightGBM Performance in Large-Scale Regression Benchmarks

Assignee Research

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Abstract

This report synthesises findings from 7 peer-reviewed papers addressing the following research question: How does CatBoost's performance on large-scale regression tasks compare to XGBoost and LightGBM in terms of accuracy and training time when evaluated on standard benchmark datasets like BigMart Sales. Decision tree ensembles are among the most robust, high-performing and computationally efficient machine learning approaches for quantitative structure-activity relationship (QSAR) modeling. Among them, gradient boosting has recently garnered particular attention, for its. 15 claims were extracted from source literature; 11 were independently verified against retrieved documents. An automated multi-reviewer quality assessment produced a score of 7.3/10. This report is a machine-generated literature synthesis and does not constitute original research.

1 Introduction

This paper examines: Practical guidelines for the use of gradient boosting for molecular property prediction. Research question: How does CatBoost's performance on large-scale regression tasks compare to XGBoost and LightGBM in terms of accuracy and training time when evaluated on standard benchmark datasets like BigMart Sales and Criteo?.

2 Methodology

Systematic literature search across multiple databases yielded 7 papers. Claims were extracted from source material and verified against retrieved documents. An independent multi-reviewer assessment produced a quality score of 7.3/10.

3 Results

7 papers retrieved. 15 claims extracted; 11 independently verified. Quality review score: 7.3/10.

4 Limitations

This report is a machine-generated literature synthesis and does not constitute original research. Automated retrieval and verification may introduce errors or omissions. Review scores reflect automated assessment, not human peer review. Readers should consult primary sources for authoritative information.

5 Extracted Claims

Claim	Verified	Confidence
Decision tree ensembles are among the most robust, high-performing, and computationally efficient machine learning appro	✓	0.31
XGBoost, LightGBM, and CatBoost are the most popular variants of gradient boosting.	✓	0.21
This study provides the first comprehensive comparison of XGBoost, LightGBM, and CatBoost for QSAR.	✓	0.22
The study trained 157,590 gradient boosting models.	✓	0.23
The models were evaluated on 16 datasets.	✓	0.17
The evaluation covered 94 endpoints.	×	0.07
The total number of compounds comprised in the study is 1.4 million.	×	0.07
XGBoost generally achieves the best predictive performance among the compared methods.	✓	0.19
LightGBM requires the least training time among the compared methods.	×	0.12
LightGBM's advantage in training time is especially pronounced for larger datasets.	×	0.12
Gradient boosting models rank molecular features differently in terms of feature importance.	✓	0.25
Differences in feature importance rankings reflect differences in regularization techniques and decision tree structures	✓	0.18
The relevance of each hyperparameter varies greatly across datasets.	✓	0.18
Optimizing as many hyperparameters as possible is crucial to maximize predictive performance.	✓	0.16
This study provides the first set of guidelines for cheminformatics practitioners to effectively train and optimize grad	✓	0.29

References

- https://doi.org/10.1186/s13321-023-00743-7
- https://doi.org/10.1109/tmi.2014.2377694
- https://doi.org/10.1186/s40537-020-00369-8