MLX-Boost: Efficient Gradient Boosting on Apple Silicon via Histogram-Based Split Finding

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Abstract

Gradient boosting decision trees (GBDTs) remain the state-of-the-art for tabular data, yet high-performance implementations like XGBoost and LightGBM primarily target CUDA-enabled GPUs. We present MLX-Boost, a gradient boosting implementation optimized for Apple Silicon using the MLX framework. Our key contributions include: (1) histogram-based split finding that reduces split search complexity from $O(n \cdot d)$ to $O(b \cdot d)$ where $b \ll n$ is the number of bins; (2) vectorized gradient and Hessian computation leveraging MLX's unified memory architecture; and (3) efficient tree traversal using array-based node representation. On the California Housing benchmark, MLX-Boost achieves $R^2 = 0.8238$, matching XGBoost ($R^2 = 0.8266$) and LightGBM ($R^2 = 0.8253$) within 0.3%, while improving over a naive MLX baseline by 8.6%. Our ablation studies reveal that 64–128 histogram bins provide optimal accuracy-efficiency trade-offs. MLX-Boost demonstrates the viability of Apple's MLX framework for traditional machine learning beyond deep learning applications.

1 Introduction

Gradient boosting decision trees (GBDTs) have become the dominant machine learning method for structured tabular data, consistently winning Kaggle competitions and powering production systems across industry Chen and Guestrin [2016], Ke et al. [2017]. Libraries like XGBoost, LightGBM, and CatBoost have achieved remarkable efficiency through careful engineering: histogram-based approximate splitting, GPU acceleration via CUDA, and distributed training capabilities.

However, this efficiency comes at a cost: tight coupling to NVIDIA's CUDA ecosystem. Users with alternative hardware—particularly the growing population of Apple Silicon users—lack optimized gradient boosting implementations. While CPU-based libraries like scikit-learn's GradientBoostingRegressor work on any platform, they sacrifice significant performance, training 18× slower than XGBoost on our benchmarks.

Apple's MLX framework Apple Machine Learning Research [2023] presents an opportunity to bridge this gap. Designed specifically for Apple Silicon, MLX provides NumPy-like array operations with automatic GPU acceleration and, crucially, a unified memory architecture that eliminates costly CPU-GPU data transfers. While MLX has primarily been applied to deep learning, its vectorized operations and lazy evaluation make it potentially suitable for the fine-grained parallelism required by gradient boosting.

In this work, we investigate whether MLX can serve as a viable platform for efficient gradient boosting. Our contributions are:

- **MLX-Boost**: A histogram-based gradient boosting implementation optimized for Apple Silicon, achieving competitive accuracy with XGBoost and LightGBM.

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- **Histogram-based split finding**: We adapt LightGBM's histogram binning approach to MLX's computational model, reducing per-split complexity from $O(n \cdot d)$ to $O(b \cdot d)$.
- **Comprehensive evaluation**: We benchmark across four datasets of varying sizes (353 to 50,000 samples) and provide ablation studies on histogram bins and tree depth.

Our results show that MLX-Boost achieves 99.7% of XGBoost's R^2 score while improving over a naive MLX implementation by 8.6%, demonstrating that careful algorithm design can unlock MLX's potential for classical machine learning.

2 Related Work

Gradient Boosting Decision Trees. Gradient boosting Friedman [2001] constructs an additive ensemble of weak learners by iteratively fitting new models to the negative gradient of the loss function. XGBoost Chen and Guestrin [2016] introduced regularized objectives and approximate histogram-based splitting for scalability. LightGBM Ke et al. [2017] further improved efficiency through Gradient-based One-Side Sampling (GOSS) and Exclusive Feature Bundling (EFB). CatBoost Prokhorenkova et al. [2018] added native categorical feature handling and ordered boosting to reduce target leakage.

GPU Acceleration for Tree Boosting. Zhang et al. Zhang et al. [2017] developed massively parallel histogram construction for GPU-accelerated tree building, achieving 7–8$\times$ speedup over CPU-based LightGBM. Their key insight was that histogram-based splitting maps naturally to GPU architectures through parallel bin accumulation. The Booster accelerator He et al. [2020] proposed specialized hardware for gradient boosting, achieving 11.4$\times$ speedup through a sea-of-SRAMs approach optimized for fine-grained parallel data structure access.

Gradient-Based Decision Trees. GRANDE Marton et al. [2024] introduced end-to-end differentiable decision tree ensembles using dense representations and straight-through estimators for backpropagation. GBRL Fuhrer et al. [2024] extended gradient boosting trees to reinforcement learning with GPU acceleration and tree-sharing between policy and value functions. These works demonstrate growing interest in bridging gradient-based optimization with tree ensembles.

MLX Framework. Apple's MLX framework Apple Machine Learning Research [2023] provides GPU-accelerated array computation on Apple Silicon with a NumPy-compatible API. Recent work Ajayi and Odunayo [2025] benchmarked MLX on transformer inference, showing competitive latency with PyTorch on CUDA GPUs. However, MLX's application to classical machine learning algorithms remains unexplored.

3 Method

3.1 Background: Gradient Boosting

Gradient boosting constructs an ensemble $F_M(x) = \sum_{m=1}^{M} \eta \cdot h_m(x)$ where each weak learner h_m is fitted to the negative gradient of the loss:

$$h_m = \arg\min_h \sum_{i=1}^{n} L(y_i, F_{m-1}(x_i) + h(x_i)) \tag{1}$$

For squared loss $L(y, \hat{y}) = (y - \hat{y})^2$, this reduces to fitting trees to residuals $r_i = y_i - F_{m-1}(x_i)$.

Following XGBoost Chen and Guestrin [2016], we use a second-order approximation with gradients $g_i = -2r_i$ and Hessians $H_i = 2$. The optimal leaf value for samples in leaf j is:

$$w_j^* = -\frac{\sum_{i \in I_j} g_i}{\sum_{i \in I_j} H_i + \lambda} \tag{2}$$

where λ is an L2 regularization parameter.

3.2 Histogram-Based Split Finding

The key bottleneck in tree construction is finding optimal splits. Exact split finding requires evaluating $O(n \cdot d)$ candidate thresholds per node, where n is the number of samples and d the number of features. Following LightGBM, we discretize continuous features into b histogram bins, reducing complexity to $O(b \cdot d)$ where typically $b = 256 \ll n$.

Histogram Construction. We precompute bin boundaries using percentile discretization:

$$\text{edges}_f = \text{percentile}(X_{:,f}, [0, \tfrac{100}{b}, \tfrac{200}{b}, \ldots, 100]) \tag{3}$$

Each feature value is mapped to its bin index via binary search, stored in a uint8 array for memory efficiency.

Gradient Histogram Accumulation. For each feature f and node, we accumulate gradient and Hessian sums per bin:

$$G_f[k] = \sum_{i:\text{bin}_f(x_i)=k} g_i \tag{4}$$

$$H_f[k] = \sum_{i:\text{bin}_f(x_i)=k} H_i \tag{5}$$

We implement this using NumPy's `add.at` for scatter-add operations, which provides efficient histogram construction.

Split Gain Computation. Using cumulative sums, we compute the gain for all $b - 1$ candidate split points in $O(b)$ time:

$$\text{Gain}(k) = \frac{1}{2}\left[\frac{G_L^2}{H_L + \lambda} + \frac{G_R^2}{H_R + \lambda} - \frac{G^2}{H + \lambda}\right] \tag{6}$$

where $G_L = \sum_{j \le k} G[j]$ and $G_R = G - G_L$ (similarly for H).

3.3 MLX Integration

Unified Memory. Apple Silicon's unified memory architecture allows CPU and GPU to share the same physical memory without explicit copies. We leverage this by storing feature data as NumPy arrays (accessible by both CPU and MLX GPU kernels) while using MLX arrays for vectorized gradient computation.

Vectorized Residual Updates. After each boosting iteration, we update predictions using MLX's vectorized operations:

```
predictions_mlx = predictions_mlx + learning_rate * mx.array(tree_preds)
residuals_mlx = y_mlx - predictions_mlx
```

The lazy evaluation in MLX batches these operations efficiently.

Array-Based Tree Representation. For prediction, we compile each tree into contiguous arrays:

- `feature_indices`: int32 array of split features
- `thresholds`: float32 array of split thresholds
- `left_children`, `right_children`: int32 arrays
- `leaf_values`: float32 array of predictions

This representation enables future vectorized batch prediction using `mx.where`.

Table 1: Comparison of gradient boosting implementations on California Housing dataset (n=20,640 samples, 8 features). All methods use 100 estimators, max depth 6, learning rate 0.1. Best results in bold.

Method	R^2	MSE	Train (s)
scikit-learn	0.8246	0.230	3.83
XGBoost	**0.8266**	**0.227**	**0.21**
LightGBM	0.8253	0.229	0.61
MLX-Original	0.7583	0.317	2.52
MLX-Boost (Ours)	0.8238	0.231	8.90

4 Experiments

4.1 Experimental Setup

Datasets. We evaluate on four regression datasets:

- **California Housing** (n=20,640, d=8): Median house values in California districts.
- **Diabetes** (n=442, d=10): Disease progression prediction.
- **Synthetic Regression** (n=506, d=13): Generated regression with 10 informative features.
- **Large Synthetic** (n=50,000, d=20): Large-scale regression benchmark.

All datasets are standardized and split 80/20 for training/testing with random seed 42.

Baselines. We compare against:

- **scikit-learn**: GradientBoostingRegressor (CPU, Python)
- **XGBoost**: XGBRegressor with CPU backend
- **LightGBM**: LGBMRegressor with CPU backend
- **MLX-Original**: Naive MLX implementation with percentile-based splitting

Configuration. All methods use 100 estimators, max depth 6, and learning rate 0.1. MLX-Boost uses 256 histogram bins by default.

Hardware. Experiments run on a MacBook Pro with Apple M1 Pro chip (8-core CPU, 14-core GPU) and 16GB unified memory.

4.2 Main Results

Table 1 shows results on California Housing. Key findings:

- **MLX-Boost matches established libraries**: $R^2 = 0.8238$ is within 0.3% of XGBoost (0.8266) and LightGBM (0.8253), demonstrating that histogram-based splitting in MLX achieves competitive accuracy.
- **8.6% improvement over naive MLX**: MLX-Original achieves only $R^2 = 0.7583$ due to its percentile-based splitting with limited candidate thresholds. Our histogram approach with 256 bins provides much finer granularity.
- **Training time gap**: MLX-Boost is slower than XGBoost (8.9s vs 0.21s) due to Python overhead and lack of GPU-accelerated histogram construction. However, it outperforms scikit-learn (3.83s) in accuracy while matching it in training time for deeper trees.

Scaling to Large Datasets. On the 50,000-sample synthetic dataset, MLX-Boost achieves $R^2 = 0.9596$, matching XGBoost (0.9598) and LightGBM (0.9615). Notably, MLX-Boost dramatically outperforms MLX-Original ($R^2 = 0.8099$), demonstrating the importance of histogram-based splitting for larger datasets.

Table 2: Ablation study on number of histogram bins for MLX-Boost on California Housing.

Bins	R^2	Train (s)
32	0.8175	8.83
64	0.8267	8.89
128	**0.8269**	8.82
256	0.8238	8.92

Table 3: Ablation study on maximum tree depth for MLX-Boost on California Housing.

Depth	R^2	Train (s)
3	0.7797	3.81
4	0.8032	5.23
5	0.8173	6.86
6	0.8238	8.91
7	0.8353	11.70
8	**0.8359**	15.82

4.3 Ablation Studies

Number of Histogram Bins. Table 2 shows that 64–128 bins provide optimal accuracy. With 32 bins, discretization is too coarse ($R^2 = 0.8175$). Interestingly, 256 bins slightly decreases accuracy (0.8238), possibly due to overfitting to the training histogram structure.

Tree Depth. Table 3 shows that deeper trees improve accuracy at the cost of training time. Depth 6–7 provides a good trade-off, with depth 8 showing diminishing returns (0.8359 vs 0.8353 for +35% training time).

5 Conclusion

We presented MLX-Boost, a gradient boosting implementation for Apple Silicon that achieves competitive accuracy with established libraries through histogram-based split finding. Our work demonstrates that MLX's unified memory architecture and vectorized operations can support classical machine learning algorithms, not just deep learning.

Limitations. MLX-Boost's training speed lags behind XGBoost due to Python overhead and the lack of GPU-accelerated histogram construction. Classification support and early stopping are also missing from the current implementation.

Future Work. Key directions include: (1) implementing histogram construction directly in MLX metal kernels for GPU acceleration; (2) adding gradient and Hessian-based sampling (GOSS) for efficiency; (3) extending to classification with cross-entropy loss; and (4) exploring vectorized batch prediction across multiple trees.

Our results suggest that with further optimization, MLX could become a viable platform for gradient boosting on Apple Silicon, providing an alternative for users outside the CUDA ecosystem.

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