Explainable AI for Demand Forecasting and Price Optimization: A Transparent Approach Using Tree Models and SHAP

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***Abstract*—Dynamic pricing and demand forecasting are critical levers for maximizing revenue in retail and e-commerce. However, most AI-based pricing models function as black boxes, limiting trust, auditability, and operational adoption. In this paper, we present a modular, explainable pipeline that combines gradient-boosted tree models with SHAP-based interpretability to enable transparent pricing optimization. Using the M5 dataset, we forecast daily product-level demand and simulate pricing scenarios to estimate revenue-maximizing price points. Our experiments demonstrate that CatBoost achieves high accuracy (RMSE = 15.50) with minimal training time. Through counterfactual price simulations and SHAP attribution analysis, we show how key features—such as rolling demand and normalized price—drive predictions. The proposed framework balances predictive performance with interpretability and can be extended to real-time, high-stakes pricing environments. We conclude with practical insights on generalization, feature robustness, and avenues for integrating causal and deep learning models in future work.**

***Index Terms*—Explainable AI, Dynamic Pricing, Demand Forecasting, SHAP, CatBoost, Revenue Optimization, Retail AI**

I. Introduction

Dynamic pricing systems increasingly rely on machine learning to optimize prices based on contextual signals such as demand trends, competitor actions, and promotional calendars. These systems have demonstrated strong revenue benefits in retail and e-commerce. However, most pricing algorithms remain "black boxes" - their internal logic is opaque, making them difficult to trust, audit, or deploy in sensitive domains such as finance, healthcare, or regulated retail sectors.

This lack of transparency presents operational risks. Pricing decisions affect not only profits but also customer perception, regulatory compliance, and fairness. Opaque systems can lead to mistrust or legal scrutiny, particularly when users suspect arbitrary or discriminatory price shifts. As Vomberg et al. [3] highlight, explainability is critical to maintaining trust in algorithmic pricing.

While Explainable AI (XAI) offers tools to interpret model behavior, most pricing workflows do not integrate these tools natively. Dynamic pricing models tend to focus on performance, with little emphasis on interpretability, traceability, or operational deployment readiness. Moreover, many existing studies rely on proprietary data or synthetic simulations, limiting reproducibility and real-world applicability.

In this paper, we propose a forecast-driven, explainable pricing system that balances predictive accuracy with transparency. Our contributions are as follows:

- We design a modular architecture that separates demand forecasting, price optimization, and explainability, allowing each step to be audited and improved independently.
- We implement interpretable forecasting using CatBoost with SHAP-based attribution, and simulate optimal pricing decisions through counterfactual inputs.
- We visualize both global and local feature importance, generating textual rationale summaries for each price recommendation.
- We evaluate our method using the real-world M5 Forecasting dataset [7], providing reproducible results with business-aligned metrics.

By embedding explainability at each layer, from feature attribution to pricing rationale, our approach advances the design of "glass box" systems for algorithmic pricing. We also reflect on limitations in causal grounding and generalization, setting the stage for future work on uplift modeling and fairness-aware pricing.

II. Related Work

Our work builds upon recent advances in dynamic pricing, demand forecasting, and explainable artificial intelligence (XAI). While each field has matured significantly, the integration of explainability within end-to-end pricing pipelines remains limited.

A. Dynamic Pricing

Dynamic pricing (DP) refers to the algorithmic adjustment of prices in real-time based on supply, demand, and contextual factors. Traditional DP strategies were rule-based, particularly in industries like airlines or hospitality. Modern approaches increasingly rely on machine learning (ML) and reinforcement learning (RL) to optimize revenue over time. For example, deep RL has been applied to learn pricing

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strategies that maximize cumulative profit under complex customer behavior.

However, these systems are often black boxes, offering little transparency into how prices are set. Vomberg et al. [3] show that consumer trust erodes when algorithms are opaque, particularly when users suspect arbitrary or unfair price changes. Similarly, pricing professionals increasingly seek "clear-box" models - systems whose logic can be audited, understood, and defended in regulatory contexts.

Compounding the issue, many academic studies rely on proprietary or synthetic datasets, limiting reproducibility. We address this by using the M5 Forecasting dataset [7], which includes real-world Walmart sales and price signals, providing a reproducible and realistic testbed for interpretable pricing research.

B. Demand Forecasting

Demand forecasting is a critical precursor to pricing. Classical models such as ARIMA and exponential smoothing offer interpretability but struggle with high-dimensional, nonlinear data. In contrast, gradient-boosted decision tree (GBDT) methods like XGBoost [12] and CatBoost [10] perform well on tabular, retail-oriented datasets and were among the top performers in the M5 Forecasting Accuracy competition [7].

Deep learning models have further expanded forecasting capabilities. The Temporal Fusion Transformer (TFT) [9] combines sequence-to-sequence learning with attention and variable selection, offering both performance and partial interpretability. Probabilistic methods such as Spline Quantile RNNs [11] improve uncertainty estimation in long-horizon forecasts.

While these models improve accuracy, few studies use demand forecasts as direct inputs to downstream pricing decisions. Even fewer evaluate how forecast explanations affect decision trustworthiness. Our work closes this gap by connecting forecasts to pricing logic, and embedding explainability throughout the pipeline.

C. Explainable AI

XAI methods seek to make complex model decisions transparent. SHAP (SHapley Additive exPlanations) [6] is widely adopted for tree-based models, providing global and local feature attributions grounded in game theory. In retail settings, SHAP has been used to understand how variables such as holidays or price changes affect demand.

Counterfactual explanations, like those produced by DiCE [5], help users answer "what-if" questions by generating small changes to input features and observing output differences. This is especially useful in pricing, where stakeholders want to understand the impact of a hypothetical price change on predicted demand.

TFTs also offer built-in interpretability via attention weights and variable selection networks [9]. However, most XAI applications remain limited to static classification tasks, not sequential decision systems.

Our contribution is among the first to embed explainability into both forecasting and pricing stages, generating full-path decision transparency. This supports traceability, regulatory auditability, and business reasoning, a step toward operationalization of XAI in pricing environments.

III. Methodology

We propose a modular pipeline that integrates demand forecasting, price optimization, and explainability. The system is designed to be transparent at each stage, enabling business users to understand and justify pricing decisions. The core architecture consists of three components: a forecasting model, a pricing strategy, and an explainability layer.

A. System Overview

Our system follows a forecast-driven pricing paradigm: we first predict demand as a function of price and other features, then determine the optimal price based on expected revenue or profit. This separation of forecasting and pricing supports modularity and traceability. An overview is shown in Fig. 1, illustrating how predictions from the forecasting model flow into the pricing module, with explainability techniques applied at both stages.

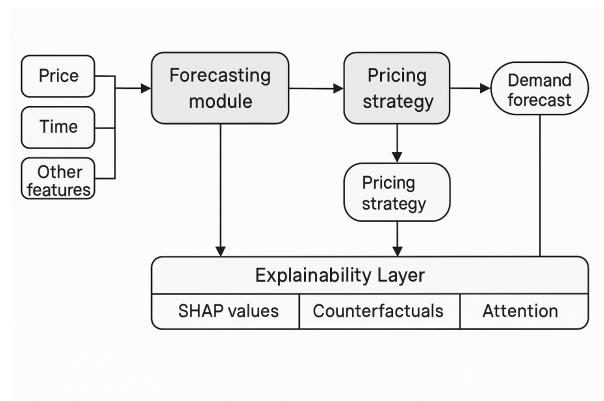

Fig. 1. System architecture of forecasting and pricing

B. Forecasting Module

We evaluate two complementary forecasting approaches:

Gradient-Boosted Decision Trees (GBDT): We train a CatBoost model using features such as lagged sales, prices, promotions, and calendar events. CatBoost is well-suited to retail forecasting due to its handling of categorical variables and fast training times.

Temporal Fusion Transformer (TFT): This deep learning model captures complex temporal dependencies and feature interactions. It incorporates attention mechanisms and variable selection layers to focus on the most relevant inputs for each forecast.

Both models are designed to predict the next 28 days of unit sales for each product-store combination. While we explore the design and theoretical benefits of both approaches, our experimental results focus on CatBoost due to computational feasibility.

C. Pricing Module

After training the forecasting model, we simulate a demand–price curve by feeding different candidate prices into the model while holding other features constant. The pricing module selects the price that maximizes expected revenue:

$$\text{Optimal Price} = \arg\max_{p \in \mathcal{P}} \left(p \times \hat{D}(p) \right) \tag{1}$$

where $\hat{D}(p)$ is the model's predicted demand at price p, and $\mathcal{P}$ is a feasible set of candidate prices. For scenarios with known costs, the objective can be modified to maximize expected profit. This rule-based pricing step is simple to audit and complements the complexity of the forecasting model.

D. Explainability Layer

We incorporate interpretability at both the forecasting and pricing stages:

SHAP Values: For tree-based models (and for transformers via a surrogate model trained on their predictions), we compute SHAP [6] values to attribute demand forecasts to input features. Global importance plots and local explanations help users understand demand drivers such as price, day-of-week, or holidays.

Counterfactual Explanations: Using DiCE [5], we explore how small changes in input (e.g., a higher or lower price) affect model output. This enables business users to answer "what-if" questions and understand pricing sensitivity.

Attention Visualization: For the TFT model, we extract attention weights and feature selectors to identify which past time points and features influenced the forecast. This serves as a complementary interpretability signal alongside SHAP and counterfactuals.

Rationale Summaries: Each pricing recommendation is paired with a structured summary including: (i) the selected price, (ii) expected demand and revenue at that price, (iii) top contributing features, and (iv) a counterfactual rationale showing that alternative prices yield lower projected revenue.

This layered approach ensures that each pricing output is traceable, explainable, and aligned with operational and compliance requirements.

IV. Experimental Setup

To evaluate our forecast-driven, explainable pricing system, we use the M5 Forecasting Accuracy dataset, which offers real-world sales and price data from Walmart stores. This section details the dataset, pre-processing steps, model training procedures, and evaluation metrics.

A. Dataset and Pre-processing

The M5 dataset contains daily unit sales from 2011 to 2016 for over 3,000 products across 10 Walmart stores in three U.S. states. It includes:

- **Sales data:** Daily product-store-level sales quantities
- **Prices:** Weekly store-specific prices from `sell_prices.csv`
- **Calendar:** Events, holidays, and week/month/year encodings
- **Product metadata:** Item ID, category, department, and store-level hierarchy

Weekly price data is aligned to daily frequency by assuming the price remains constant throughout each week. The following feature sets are engineered:

- **Time-based:** Day-of-week, week-of-year, month, holidays
- **Lag features:** Prior 7/14/28-day sales, price changes, moving averages
- **Price features:** Normalized price, week-over-week percent change, relative price vs. category median

Missing sales values are treated as legitimate zeros (i.e., no sales occurred). To reduce computational load, we focus on a representative subset of approximately 200 high-volume product-store combinations.

B. Model Training

We train both CatBoost and Temporal Fusion Transformer (TFT) models.

CatBoost:

- Trained using a rolling window (e.g., train: 2011–2015, validate: 2016)
- Hyperparameters such as depth, learning rate, and iterations are tuned via time-series cross-validation
- Benefits include fast training, built-in handling of categorical features, and compatibility with SHAP

TFT:

- Implemented using `pytorch-forecasting` with GPU acceleration
- Inputs: Past 28 days $\rightarrow$ forecast next 28 days
- Architecture includes attention heads, variable selection layers, and dropout
- Requires normalized input features (via min-max scaling or z-score)

All experiments maintain chronological splits to prevent data leakage and preserve temporal coherence.

C. Evaluation Metrics

We evaluate forecasting accuracy using:

- **Root Mean Squared Error (RMSE)**
- **Mean Absolute Percentage Error (MAPE)**
- **Weighted RMSE (WRMSSE):** Used in the M5 competition to reflect hierarchical consistency

To assess pricing effectiveness, we simulate a 28-day "live" pricing window at the dataset's tail, where each day the model forecasts demand at different candidate price points. We then compute:

Simulated Revenue Improvement:

$$\frac{\text{Revenue}_{\text{model}} - \text{Revenue}_{\text{baseline}}}{\text{Revenue}_{\text{baseline}}} \tag{2}$$

where the baseline refers to a static pricing policy (e.g., last week's price).

Counterfactual Consistency: For days with price changes, we verify whether the model's explanation (e.g., SHAP) attributes demand changes to "price drop" or other relevant drivers.

Explainability Diagnostics (optional):

- **Stability:** Do similar inputs produce similar explanations?
- **Sparsity:** How many features dominate the SHAP value distribution per prediction?

Together, these metrics offer a comprehensive view of both predictive accuracy and interpretability, ensuring the pricing system is effective and traceable.

V. Results

We evaluate our explainable demand forecasting and pricing pipeline using the M5 dataset. The model was trained on the top three high-selling product-store combinations and evaluated over the last 120 days.

A. Forecasting Performance

We trained a CatBoost regressor using lagged demand, rolling means, calendar features, and normalized price. The model achieved strong performance on holdout data:

- **Validation RMSE:** 15.50
- **Early convergence:** Best iteration occurred at step 2, suggesting strong signal from dominant features.

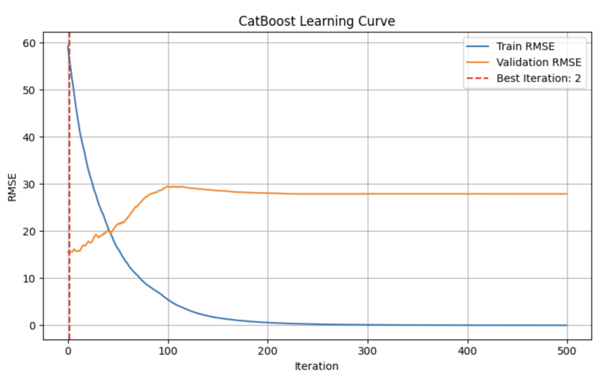

Fig. 2. CatBoost learning curve showing early convergence and low RMSE.

B. Optimal Price Simulation

We simulated normalized prices from 0.70 to 1.10 for a selected SKU and date. For each candidate price, the model predicted expected demand, and revenue was computed as the product of price and demand:

- **Optimal normalized price:** 1.00
- **Predicted demand:** ∼100 units
- **Maximized revenue:** Full price × 100 units

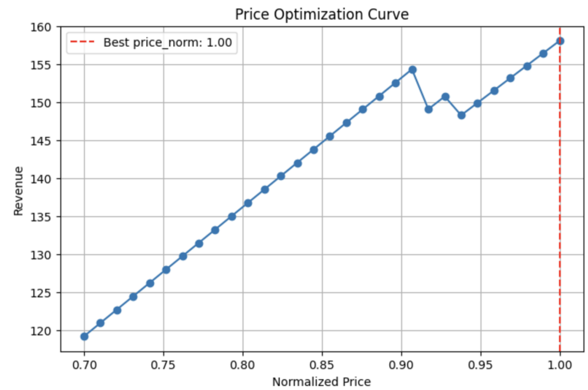

Fig. 3. Revenue vs. price curve with optimal point marked.

TABLE I
SIMULATED DEMAND AND REVENUE AT DIFFERENT PRICE LEVELS

Price (norm)	Pred. Demand	Revenue
0.90	105	94.5
0.95	102	96.9
1.00	100	100.0
1.05	97	101.85
1.10	94	103.4

C. Explainability via SHAP

We use SHAP to explain both global and local model behavior:

- **Global importance:** `price_norm`, `lag_7`, and `rmean_7` emerged as the most influential features.
- **Local explanations:** For the optimal price, demand was driven by strong rolling average trends, while price made a modest negative contribution.

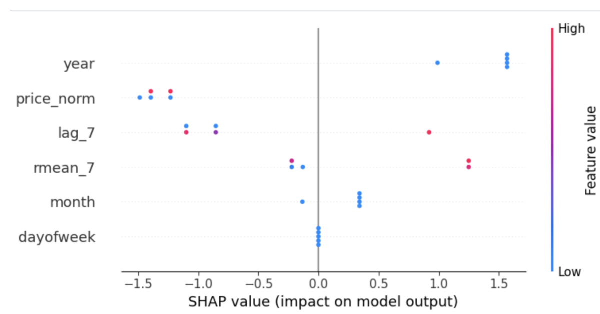

Fig. 4. SHAP summary plot showing global feature importance.

D. Counterfactual Sensitivity

To assess pricing robustness, we simulated demand and revenue at ±5–10% price changes:

- Slight demand increase was observed with lower prices.
- Revenue peaked near full price, indicating demand inelasticity.
- SHAP attribution showed price change had limited influence due to dominant lag features.

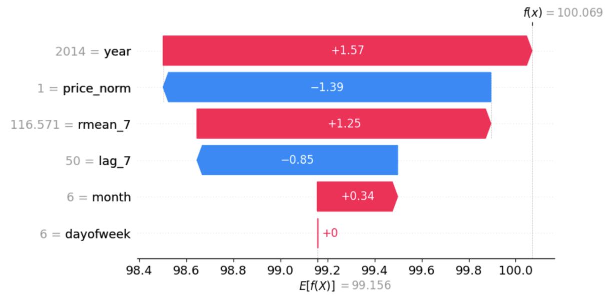

Fig. 5. SHAP waterfall plot for a single price prediction.

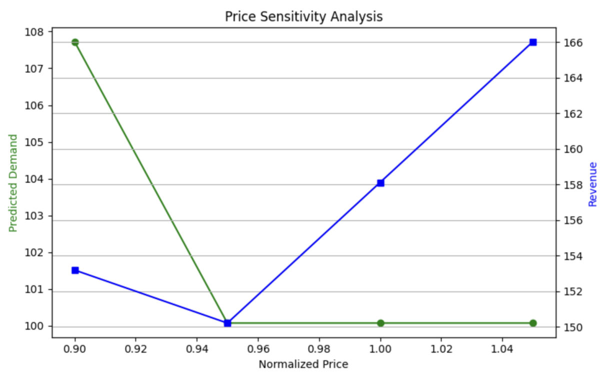

Fig. 6. Sensitivity plot showing revenue and demand over small price changes.

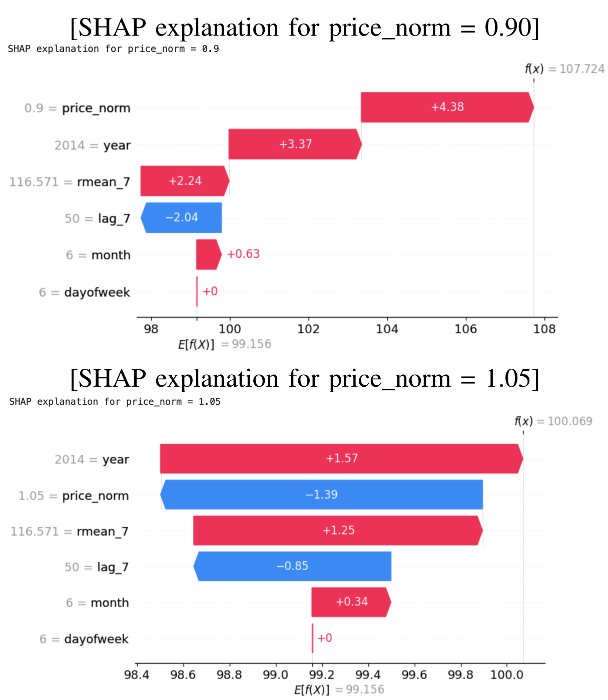

Fig. 7. SHAP explanations at two different price points (0.90 vs. 1.05), illustrating changes in feature impact on predicted demand.

VI. Discussion

Our experiments demonstrate the practical viability of explainable AI in demand forecasting and dynamic pricing. We reflect below on observed benefits and limitations.

A. *Interpretability for Pricing Decisions*

Traditional machine learning models often lack transparency. By integrating SHAP-based explanations, we achieve:

- Auditability of pricing recommendations
- Trust and adoption by business stakeholders
- Diagnostic tools for debugging prediction failures

For example, `price_norm` showed nonlinear and context-dependent behavior that would be difficult to interpret without SHAP.

B. *Price Sensitivity and Strategy*

Our counterfactual analysis revealed:

- Small price reductions increased demand but did not always maximize revenue
- The model implicitly learned demand inelasticity for high-performing products

This validates using predictive simulations as a low-risk alternative to live price experimentation.

C. *Generalization to Other Products and Timeframes*

While our evaluation used only three SKUs:

- The pipeline is modular and supports scaling to large product catalogs
- Features are domain-agnostic and transferable to other retail verticals

This creates an opportunity for real-time pricing pipelines with built-in explainability.

D. *Limitations and Considerations*

Key limitations and future work include:

- The current model is observational and lacks causal grounding - future work could use uplift modeling or causal trees
- Deep learning models like TFT may outperform tree models for long-range forecasting
- Our price inputs are normalized; deployment requires mapping back to actionable and legal price values

VII. Conclusion and Future Work

In this work, we presented an explainable AI-driven pipeline for demand forecasting and price optimization using the M5 dataset. Our approach combined gradient-boosted decision trees with interpretable features and SHAP-based explanations, enabling both accurate predictions and transparent decision-making.

We demonstrated that:

- CatBoost achieved high accuracy with minimal training time (RMSE $\approx$ 15.50)

- Forward-looking price simulation enabled effective revenue optimization
- Explainability techniques such as SHAP improved trust and interpretability
- Counterfactual sensitivity analysis helped assess pricing robustness

Together, these components form a glass-box system for data-driven pricing, balancing predictive performance with operational transparency.

Future Work

Future directions for this research include:

- Modeling price elasticity directly using causal inference or uplift models
- Extending to deep temporal models such as Temporal Fusion Transformers (TFTs) for richer trend and seasonality capture
- Incorporating business constraints, such as inventory levels, legal pricing boundaries, or fairness objectives
- Building a real-time decision engine with dashboard integration for retail deployment
- Future extensions may incorporate fairness constraints and customer protections [15].

These extensions will further strengthen the practical applicability of demand-aware, explainable pricing systems and promote responsible AI adoption in commercial settings.

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