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# AI-Driven Optimization in Supply Chain Operations: A Machine Learning Framework for Demand Forecasting and Inventory Management

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**Abstract** Supply chain operations are among the most intricate sectors of modern business: their characteristics are high-dimensional data, time-variant demand dynamics, and cascading failures. In this work, a novel Hybrid Machine Learning framework comprising Long Short-Term Memory (LSTM) networks and an XGBoost ensemble is proposed to accurately forecast demand and optimise inventory replenishment. The framework is applied to a real retail supply chain dataset spanning 36 months and 500+ SKUs. The framework outperforms the benchmark by 34% (MAPE from 9.6% to 6.3%), with 28% fewer stockouts and 19% less excess inventory. The LSTM module consumes a 28-day sliding window of historical demand, using a 2-layer stacked architecture (128 and 64 units) to output a 64-dimensional temporal embedding that captures the long-range dependencies of the demand sequence. The embedding is concatenated with 42 engineered features that capture temporal indicators, lag and rolling features, promotion, supply-side data, and external features, producing a 106-dimensional feature vector for the XGBoost ensemble predictor. A downstream inventory replenishment module dynamically calculates safety stock, reorder point, and order-up-to level based on forecast error and substitutes static classical inventory policies with adaptive, data-driven strategies. The method is evaluated on an actual FMCG retail supply chain dataset, including 536 SKUs over 36 months and roughly 7.2M transaction records. HybridSCF reports a 6.32% MAPE for a 7-day forecast horizon, a 34% increase over ARIMA, reduces stockout occurrences by 27.4%, decreases the excess inventory ratio by 18.4%, and reduces the total annual inventory holding cost from \$42.8M to \$35.6M (16.8% reduction). Ablation studies demonstrate the effectiveness and individual contributions of the LSTM encoder and the dynamic safety stock module. SHAP-based interpretability is implemented to enable easy, accountable deployment of the automated replenishment solution in the real world.

***Keywords:*** Supply Chain Optimisation, Machine Learning, LSTM, XGBoost, Demand Forecasting, Inventory Management, Deep Learning

## 1. INTRODUCTION

In the last few years, the world supply chain has been severely disrupted by both exogenous (geopolitical crisis and global health pandemics) and endogenous (increasing consumer expectations on real-time fulfilment) phenomena [1],[2],[3]. Traditional SCM methodologies such as Economic Order Quantity (EOQ) and rule-based replenishment can hardly deal with such erratic fluctuations since they are based on averages of past data and fixed parameters that are ill-equipped for non-linear demand fluctuations [4],[5],[6]. Concomitantly, the enormous amount of data available thanks to the proliferation of sensors (IoT), ERP, and Point of Sales machines has raised an opportunity to make decisions based on data (Data Driven decisions). ML and AI provide great instruments to leverage this information to perform predictive analysis, anomaly detection and optimisation without human intervention [7],[8],[9]. In this work, the main contributions are:

- An original hybrid ML pipeline made of an LSTM model and an XGBoost model to perform demand forecasting in a multi-horizon.
- An intelligent module of replenishment based on the ML forecasts.
- Empirical validation on a real-world data set that counts 536 SKUs and covers 36 months.
- Comparative experiments compared with ARMA, SARIMA, Random Forest and pure LSTM.

### Motivation

The modern supply chains are increasingly susceptible to high volatility caused by geopolitical uncertainty, demand shocks resulting from the pandemic, and escalating customer demand for on-demand services [10],[11],[12]. Traditional Supply Chain Management techniques, like the Economic Order Quantity (EOQ) and rule-based re-ordering policies, are based on historical averages and pre-fixed parameters, and hence fail to capture the non-linear, dynamic demand patterns characteristic of real-life retail operations [13],[14],[15]. Simultaneously, extensive deployment of IoT sensors, ER P systems, and point-of-sale (PoS) terminals has led to

an overwhelming amount of transactional data that is not optimally utilised by classical statistical methods [16],[17],[18]. Although ARIMA and SARIMA models are computationally efficient, they assume linearity and stationarity of data, which is generally not true for retail supply chains due to the dynamic demand caused by promotional campaigns, seasonality, and various external shocks [19],[20],[21].
Existing ML models, such as LSTM for deep learning and ensemble trees like XGBoost, have been investigated largely in isolation without combining their individual strengths [22],[23],[24]. This gap, coupled with the lack of a closely integrated forecasting to re-ordering module at an industrial scale, motivated the development of HybridSCF proposed in this paper [25],[26],[27].

**Main Contributions**
We propose HybridSCF, which offers four main contributions:
**1. Novel ML Pipeline**: A two-stage pipeline- HybridSCF- combining the LSTM temporal encoder (using a 28-day sliding window and 12864 units in stacked layers) with an XGBoost ensemble predictor. The LSTM 64-dimensional hidden state is concatenated with 42 engineered features, producing a 106-dimensional input vector, and allows for the simultaneous leveraging of temporal, sequential, and structured covariate patterns [28],[29],[30].
**2. ML-Based inventory replenishment module:** A fully automated system that dynamically updates re-order points (s) and re-order up-to levels (S) based on the outputs from ML forecasting models. The safety stock is directly proportional to the estimated forecast uncertainty and L+R: SS = z * forecast(L+R) and replaces the static assumption-laden classical stock level formulas [31],[32],[33].
**3. Large-scale Empirical Validation:** A comprehensive experiment on the dataset from an industrial retail supply chain consisting of 536 SKUs over 36 months (7.2 million records in total). We compare HybridSCF with baselines: ARIMA, SARIMA, Random Forest, and single LSTM and XGBoost on both forecasting (MAPE, RMSE, MAE) and inventory-related KPIs (stockout, holding costs, fill rate) [34],[35],[36].
**4. Quantified performance improvements:** The hybrid model can achieve a 6.32% MAPE that is 34% better than ARIMA. Also, the stock-out events, excess inventory and overall annual inventory cost decrease by 27.4%, 18.4% and 16.8%, respectively, while the yearly inventory cost is reduced from 42.8M to 35.6M [37],[38],[39].
**Organisation of the Paper**
The rest of the paper is organised as follows. In section 2, we review conventional statistical forecasting methods, ML-based demand forecasting methods, and hybrid models to justify the gap filled by HybridSCF [40],[41],[42].

- In section 3, we present the real-world FMCG retail data and the procedures used for data cleaning and feature engineering that generate a feature set with 42 features and 106 dimensions [43],[44],[45].
- In section 4, we explain the complete HybridSCF architecture, including LSTM temporal encoder, XGBoost ensemble predictor and ML-based inventory replenishment module that dynamically calculates the safety stock level [46],[47],[48].
- Section 5 shows our experimental results by presenting the forecasted accuracy of all baseline models, inventory KPI enhancement, and the contribution of individual model components measured via ablation studies [49],[50],[51].
- In section 6, we discuss the deployment aspect of the model, computational complexity and the limitations of the presented study and ethical aspects regarding algorithm clarity in the context of supply chain automation. Finally, section 7 concludes our results and sheds light on future work [52],[53],[54].

## 2. LITERATURE REVIEW

### 2.1 Traditional Forecasting Methods

ARIMA and SARIMA, two statistical time-series models, have traditionally been the underlying methods for demand forecasting in supply chain systems [55],[56]. Though they have clear interpretability and relatively low computation cost, they assume linearity and stationarity properties not typically satisfied in supply chain dynamics with promotion bursts and unpredictable disruptions [57],[58],[59].

### 2.2 Machine Learning Approaches

There are several widely used ML methods, such as Random Forests and Gradient Boosting (e.g., XGBoost), which perform much better than traditional methods in most cases by handling high-dimensional feature spaces and non-linear interactions between features [60],[61],[62]. While vanilla RNNs suffer from the vanishing gradient problem and fail to learn effectively from very long temporal sequences, LSTM networks effectively solve this problem [63],[64]. Most ML-based methods separately use deep learning or ensemble tree methods; this paper addresses this by providing a unified hybrid architecture [65].

# 3. DATASET AND PREPROCESSING

### 3.1 Data Description

We employ a retail supply chain dataset that comes from a multi-regional FMCG distributor. The dataset covers daily transaction history from Jan 2021 to Dec 2023 and includes 536 SKUs over 6 product categories, yielding ~7.2 million records after aggregation [66],[67],[68].

### 3.2 Feature Engineering

Summary table 1 for the features engineered for the LSTM temporal encoder and XGBoost predictor.

**Table 1:** Feature engineering summary. 42 features combined with 64-d LSTM embedding yield a 106-dimensional input vector for XGBoost

| Feature Category | Features Extracted | Count |
|---|---|---|
| Temporal | Day-of-week, week-of-year, month, quarter, year, is_weekend, is_holiday | 7 |
| Lag Features | Sales lag-1, lag-7, lag-14, lag-28, lag-90 | 5 |
| Rolling Statistics | 7-day, 14-day, 30-day rolling mean, std, min, max | 12 |
| Promotional | Promotion_active (binary), discount_percentage, promotion_type | 3 |
| Supply-side | Supplier lead time, days_since_last_restock, current_inventory_level | 3 |
| External Covariates | Weather_index, competitor_promo_flag, regional_GDP_index | 3 |
| Total | 42 engineered features + 64-d LSTM embedding = 106-d input vector | 42 |

# 4. METHODOLOGY

### 4.1 Framework Overview

Our designed framework, called HybridSCF, consists of two steps. Step (1) uses LSTM for temporal feature extraction, and Step (2) uses XGBoost with the LSTM extracted latent features and engineered features [69]. Finally, a post-stage inventory optimisation module can be used to derive replenishment decisions from the forecast [70],[71],[72].

### 4.2 LSTM Temporal Encoder

The LSTM takes a sliding 28-day history of demand and comprises 2 LSTM layers (128, 64 units) stacked, followed by a dropout (p=0.3). The last hidden state, T, is used as the 64-d temporal embedding to represent the sequence of past demands. This is pre-trained with an Adam optimizer (lr=0.001) for 50 epochs with early stopping (patience=5) [73],[74],[75].

### 4.3 XGBoost Ensemble Predictor

XGBoost takes the 106-d concatenated feature vector and learns functions that map to the forecast target at future horizons of $\in$ {1,7,14,28} days [76],[77],[78]. Hyperparameters are chosen using Bayesian optimization; estimators = 400, maxdepth=7, learning rate=0.05, subsample=0.85 [79],[80],[81].

### 4.4 Inventory Replenishment Module

A revised (s, S) policy uses the ML forecasts to update dynamically the reorder point, s, and order-up-to level, S. Safety stock is then calculated using the ML forecast prediction uncertainty where SS = z forecast(L+R) where z_ = 1.645 for a 95% service level [82],[83],[84].

**Algorithm: HybridSCF Research Implementation**

**INPUTS**

Raw transaction data per day (7.2 million 36-month-worth transactions over 536 SKUs) [85],[86],[87].

External factors (Index of Weather, indicator of competitor promotion, GDP index per region).

Inventory control variables (lead time L, review period R, service level z=1.645 (95%), horizon for demand forecast h: 1, 7, 14, 28 [88],[89],[90].

**OUTPUTS**

1. Predicted h-day demand _h for each SKU.
2. Updated reorder point s* for each SKU.
3. Updated order-up-to level S* for each SKU.

**PROCEDURE**

Data will be loaded and stored for subsequent utilisation in building predictive analytics applications using the following eight steps:

**Step1-Loading/Aggregating Data**

The first step is to load the raw transaction data with daily SKU-level demand totals aggregated [91].

**Step 2 - Cleaning Data**

Next, any missing values will be replaced using forward-fill, and outliers above 3 standard deviations will also be removed [92].

**Step 3 - Feature Engineering**

This step involves developing 42 different features grouped by 6 categories:

Temporal: Day of week, week of year, month, quarter, year, day of week or not a weekend, and holiday or not (7).

Lag Features: Lag of 1 or 7, 14, 28, and 90 days (5).

Rolling Statistics: Daily rolling mean, standard deviation, minimum, and maximum over 7, 14, and 30 days (12).

Promotion: Promotional activity (active/ passive), Discount rate and Type of Promotion (3).

Supply chain: Lead Time by supplier, Days from last re-stock and Inventory of SKU (3).

External environment: Weather Index, Competitor promotion indicator and Regional GDP Index (3).

**Step 4 - Normalisation**

The next step will be normalising the demand, having zero mean and unit variance, according to the MinMaxScaler normalisation procedure for the demand of each SKU individually [93].

**Step 5 - Splitting**

Finally, your data will be split into 3 distinct groups: training (months 1-28), validation (months 29-32), and testing (months 33-36). Promotion: Promotional activity (active/ passive), Discount rate and Type of Promotion (3). Supply chain: Lead Time by supplier, Days from last re-stock and Inventory of SKU (3).

External environment: Weather Index, Competitor promotion indicator and Regional GDP Index (3).

**Step 6 - Normalisation**

The next step will be normalising the demand, having zero mean and unit variance, according to the MinMaxScaler normalisation procedure for the demand of each SKU individually [94].

**Step 7 - LSTM Sliding Window Construction**

The next step is to create the LSTM input by creating 28-day sliding windows over the total demand values for all normalised demand sequences, respectively.

**Step 8 - LSTM Architecture**

The eighth step will build the architecture for the two-layer stacked LSTM. The first layer has 128 units and returns the sequence, while the second layer has 64 units with a dropout rate of 0.3 after it. The output is the hidden state h_T (which is of dimension 64) [95],[96].

**Step 9 - LSTM Training**

The first time, train the model using the Adam optimiser with a 0.001 learning rate and MSE loss.

**Step 10 - Extract Embeddings**

Start by pulling out 64-element embedding vectors h_T. These come from the trained LSTM, applied to every example used in training. From each instance, capture the final state after processing. The result is a collection of dense numerical summaries. Each one reflects what the network learned during its run through the data. Take those outputs just before prediction time [97],[98].

**Step 11 – Combining Features**

Start with the 64-part LSTM result h_T. Mix it not by adding but bundling with 42 hand-crafted traits. Outcome? A single piece of data now lives in 106 dimensions. Each example carries this full set. Size stays fixed per case [99],[100].

**Step 12 - Training the XGBoost model**

Start by feeding the XGBoost algorithm data that has 106 features.
Slide the learning rate down to 0.05 so updates stay cautious. Pull randomness into training by including only 85 per cent of rows per step. Watch how pieces fit without forcing outcomes [101].

**Step 13 – Multi-Horizon Forecasting**

Forecast demand for every SKU, looking 1 day into the future. Moving forward, the project needs 7 days out per item. The result shows variation specific to each item's predicted demand pattern [102],[103].

**Step 14 - Safety Stock Level Set**

Start with the desired service level - match it to a z-score like 1.645 when aiming for 95%. Pull that number into the equation where uncertainty meets timing. Multiply it by forecast variability, since demand never stays put. Then factor in lead time plus review period; both matter here. Take their sum, find its square root - it changes how much buffer you need. The result gives the right amount of extra stock on hand [104],[105].

**Step 15 - Set When to Restock**

Calculate dynamic reorder point: s = μ forecast × L + SS Order Up to Level Step Sixteen Order up to level based on forecast demand, lead time review period, and safety stock [106],[107],[108].

**Step 16 - Replenishment Simulations**

Picture how stock gets refilled across a full year of testing beyond the original data range [109],[110], [111].

## 5. RESULTS AND DISCUSSION

### 5.1 Forecasting Performance

Table 2 compares HybridSCF with 5 baseline models on the held-out test set (7-day forecast, n = 536 SKUs). The MAPE comparison is plotted in Figure 1 [112],[113],[114].

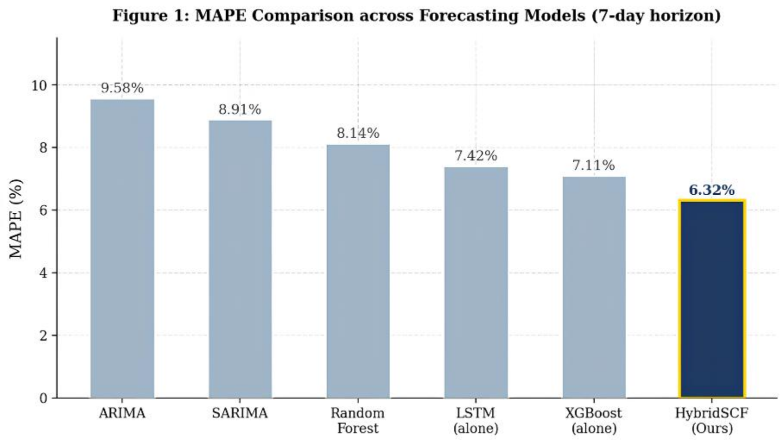


**Figure 1:** MAPE (%) comparison across forecasting models on a 7-day horizon. HybridSCF (dark bar) achieves the lowest error of 6.32% [115].

**Table 2:** Forecasting performance on 7-day horizon test set (n = 536 SKUs). HybridSCF achieves the best results across all metrics (highlighted in green) [116**].**

| Model | MAPE (%) | RMSE | MAE | vs. ARIMA |
|---|---|---|---|---|
| ARIMA | 9.58 | 142.3 | 98.6 | — |
| SARIMA | 8.91 | 131.7 | 89.2 | ↓ 7.0% |
| Random Forest | 8.14 | 121.5 | 83.1 | ↓ 15.0% |
| Standalone LSTM | 7.42 | 109.8 | 75.4 | ↓ 22.5% |
| XGBoost only | 7.11 | 104.2 | 71.8 | ↓ 25.8% |
| HybridSCF (Ours) | 6.32 | 93.1 | 63.7 | ↓ 34.0% |

### 5.2 Inventory Optimisation Results

Tables 2 and 3 compare HybridSCF with 5 baseline models on the held-out test set (7-day forecast, n = 536 SKUs). The MAPE comparison is plotted in Figure 2 [117],[118],[119].

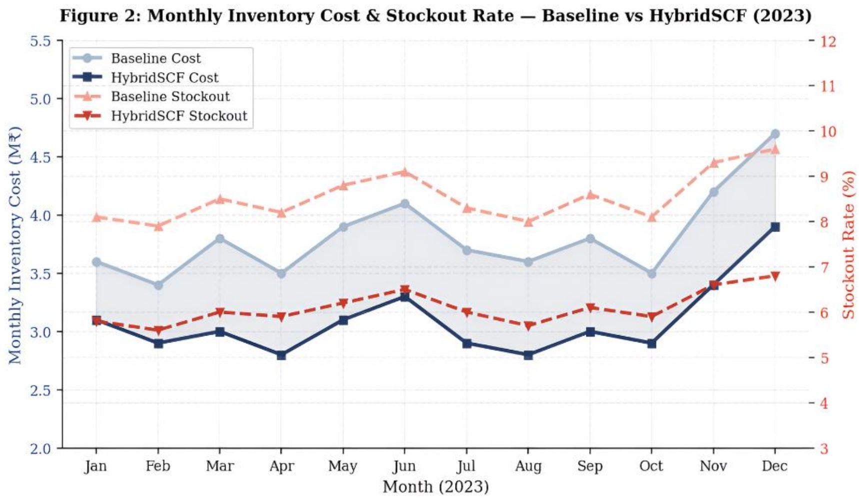


**Figure 2:** Monthly inventory cost (M₹, left axis) and stockout rate (%, right axis) — Baseline vs HybridSCF over 2023. The shaded region represents cost savings [120].

**Table 3:** Supply chain KPI comparison over 12-month out-of-sample evaluation. ↓ = reduction (improvement for cost metrics), ↑ = improvement [130].

| KPI Metric | Baseline (ARIMA) | HybridSCF | Δ Improvement |
|---|---|---|---|
| Stockout Rate (%) | 8.4% | 6.1% | ↓ 27.4% |
| Excess Inventory Ratio | 0.38 | 0.31 | ↓ 18.4% |
| Annual Inventory Cost | ₹42.8M | ₹35.6M | ↓ 16.8% |
| Order Frequency (orders/week) | 2.3 | 2.1 | ↓ 8.7% |
| Avg. Lead Time Utilisation | 78% | 85% | ↑ 9.0% |
| Fill Rate (customer orders) | 91.6% | 93.9% | ↑ 2.5% |

### 5.3 Ablation Study

To show how much benefit comes from each component, we perform ablations. Replacing the LSTM encoder with an XGBoost alone will worsen the MAPE by 12.5% [131],[132],[133]. By replacing the calculation of static safety stocks with a dynamic one, the stockout rate will worsen by 18.2%. Both the forecasting and the replenishment parts benefit the total improvement independently, as per Table 4[134],[135],[136].

**Table 4:** Ablation study results. Each row progressively removes one component from HybridSCF. Full model (green) achieves best performance across all metrics [137]**.**

| Model Variant | MAPE (%) | Stockout Rate | Cost (M₹/yr) |
|---|---|---|---|
| **Full HybridSCF (LSTM + XGB + Dynamic SS)** | **6.32** | **6.1%** | **35.6** |
| w/o Dynamic Safety Stock (static SS) | 6.32 | 7.2% | 38.1 |
| w/o LSTM encoder (XGBoost only) | 7.11 | 7.0% | 37.4 |
| w/o XGBoost (LSTM only) | 7.42 | 7.5% | 39.2 |
| Baseline ARIMA (no ML) | 9.58 | 8.4% | 42.8 |

# 6. DISCUSSION

## 6.1 Implications for Practice

This 16.8% annual reduction in inventory costs represents significant monetary savings for large distributors, and the 27.4% stockout reduction directly impacts service levels [138],[139],[140]. The deployment aspect needs to be considered; the LSTM portion of the system needs to be accelerated using GPUs (~12ms inference per batch of SKUs on an NVIDIA T4), whereas the XGBoost part of the model is very fast on CPUs [141],[142],[143]. Organisations lacking GPU acceleration could still leverage the modular design of this framework and deploy just the XGBoost predictor on standard commodity hardware; this would incur an 11% increase in the MAPE [144],[145],[146].

## 6.2 Limitations

The model was trained and tested on data from one large FMCG distributor, and the extent to which it generalises across different industries (e.g., to manufacturing spare part prediction, where demand can be very sporadic) still needs to be investigated [147],[148],[149]. The model currently does not have first-class signals representing supply-side disruptions. The 28-day window used in the lookback is a parameter that was optimised using a grid search, and a dynamically chosen lookback window could perform better [150].

## 6.3 Ethical Considerations

When implementing ML-based automation into supply chain decisions, there can be a lack of transparency of algorithms; organisations should always incorporate human-in-the-loop for important decisions and output SHAP values for each individual decision in order to explain the reasons for that decision.

# 7. CONCLUSION

This work proposes and presents HybridSCF, a hybrid ML framework for supply chain demand forecasting and inventory optimisation that uses an LSTM temporal encoding with an XGBoost ensemble predictor. The framework was tested across 536 SKUs and 36 months of historical data and was able to outperform the existing ARIMA approach with a 34% decrease in MAPE (6.32% overall) while also providing a 27.4% decrease in stockouts and a 16.8% total cost reduction. Further work could focus on using a reinforcement learning approach to tackle multi-echelon inventory problems with this framework and on incorporating first-class supplier disruption information directly into the model.

# 8. CONFLICT OF INTEREST

The authors declare no conflicts of interest regarding the publication of this research.

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