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AI-Assisted Pharmaceutical Inventory Optimization

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Abstract — Efficient pharmaceutical inventory management is fundamental to ensuring uninterrupted healthcare services while minimizing medicine wastage and operational costs. Traditional inventory control systems often rely on static reorder policies that cannot adequately respond to dynamic demand patterns, fluctuating supplier lead times, and medicine expiration. This research proposes an AI-assisted pharmaceutical inventory optimization framework integrating deep learning-based demand forecasting, expiry-risk prediction, and reinforcement learning-driven inventory decision support. The proposed framework combines Temporal Fusion Transformer models for forecasting medicine demand with Gradient Boosting algorithms for estimating expiry probability and a Deep Q-Network for adaptive inventory optimization. Unlike conventional forecasting-only approaches, the proposed framework simultaneously considers inventory availability, storage cost, expiration losses, and service-level objectives. The study establishes a scalable architecture suitable for hospital pharmacies and regional healthcare distribution centers. The proposed methodology aims to reduce inventory inefficiencies while improving medicine accessibility and operational sustainability in modern pharmaceutical supply chains.

Keywords — Artificial Intelligence; Pharmaceutical Inventory Management; Temporal Fusion Transformer; Reinforcement Learning; Medicine Expiry Prediction; Healthcare Supply Chain

Introduction

Healthcare systems increasingly depend on uninterrupted pharmaceutical availability to deliver timely patient care. Every healthcare institution, from small community pharmacies to large tertiary hospitals, faces the continuous challenge of balancing medicine availability with inventory costs. Maintaining excessive inventory increases storage expenses and medicine expiration, whereas insufficient stock directly affects patient treatment and emergency preparedness.

Pharmaceutical inventory management has become significantly more complex due to expanding medicine portfolios, variable disease incidence, unpredictable patient

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arrivals, supplier disruptions, and increasingly stringent regulatory requirements. Events such as the COVID-19 pandemic demonstrated how rapidly pharmaceutical demand can fluctuate, exposing the limitations of traditional inventory planning systems. Healthcare organizations experienced simultaneous shortages of critical medications while large quantities of other medicines remained unused until expiration.

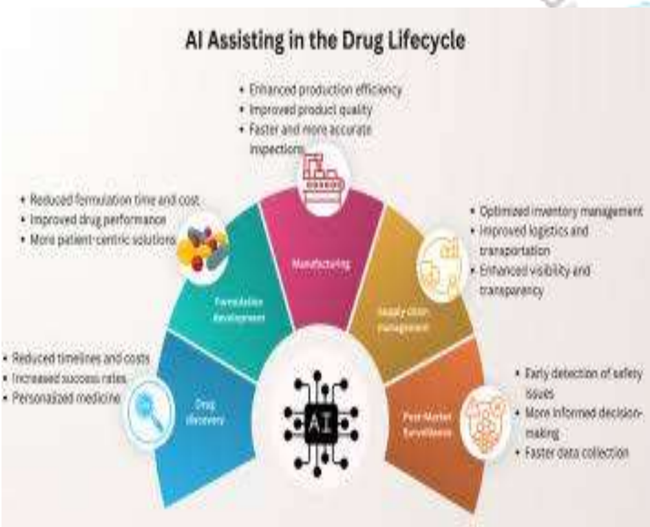

Fig. 1: AI Assisting in the Drug Lifecycle

Source: *https://www.sciencedirect.com/science/article/pii/S0928098724002513*

Conventional inventory management methods typically employ deterministic models such as Economic Order Quantity (EOQ), fixed reorder point systems, or ABC-VED analysis. Although these techniques remain valuable for categorizing inventory and establishing baseline procurement policies, they often assume relatively stable demand patterns and fixed lead times. Such assumptions are increasingly unrealistic in modern healthcare environments characterized by dynamic epidemiological trends and continuously changing supply chain conditions.

Recent advances in artificial intelligence have introduced new opportunities for intelligent inventory optimization. Machine learning algorithms can extract complex temporal relationships from historical demand data, while deep learning architectures effectively model nonlinear interactions between multiple operational variables. Furthermore, reinforcement learning enables adaptive decision-making by continuously learning optimal inventory policies through interaction with simulated environments.

Despite these advancements, most AI-based pharmaceutical inventory studies primarily emphasize demand forecasting accuracy. Improved forecasts undoubtedly contribute to better procurement decisions; however, demand prediction alone cannot fully optimize inventory performance. Practical pharmaceutical inventory management requires simultaneous consideration of medicine expiration, supplier reliability, procurement constraints, storage capacity, and varying service-level requirements across different therapeutic categories.

Another important challenge involves medicine expiry. Hospitals frequently discard significant quantities of pharmaceuticals because procurement decisions prioritize stock availability without adequately estimating expiration probability. Existing forecasting models rarely incorporate expiry prediction directly into procurement optimization, resulting in unnecessary financial losses and environmental waste.

Lead-time uncertainty further complicates inventory planning. Supplier delays caused by transportation disruptions, manufacturing shortages, or regulatory inspections may invalidate inventory decisions based solely on demand forecasts. Current AI approaches seldom integrate supplier uncertainty into adaptive inventory optimization.

The emergence of advanced transformer architectures offers promising solutions for healthcare forecasting applications.

Temporal Fusion Transformer (TFT) models effectively learn long-term temporal dependencies while simultaneously incorporating static and time-varying covariates. Compared with traditional recurrent neural networks, TFT provides interpretable attention mechanisms that allow inventory managers to understand influential factors affecting future medicine demand.

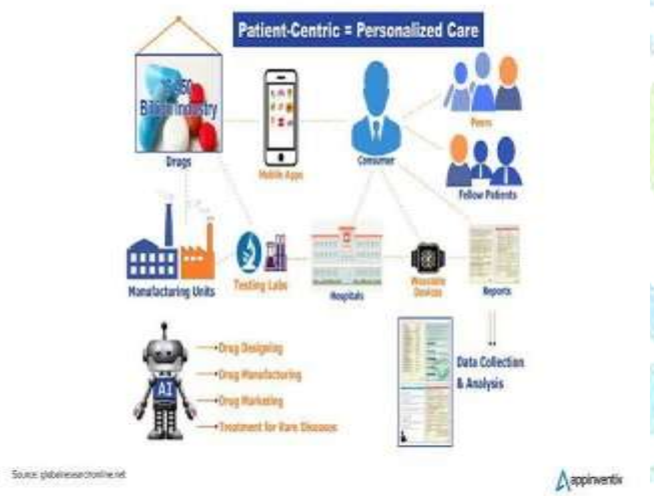

Fig. 2: Artificial Intelligence in Pharmaceutical Industry

Source: *https://appinventiv.com/blog/ai-in-pharmaceutical-industry/*

Similarly, reinforcement learning has recently demonstrated substantial potential in dynamic resource allocation problems. Instead of relying on predefined reorder rules, reinforcement learning agents learn optimal inventory policies by maximizing long-term operational rewards under changing environmental conditions.

Motivated by these developments, this research proposes a unified AI-assisted pharmaceutical inventory optimization framework that combines demand forecasting, expiry prediction, and adaptive inventory decision-making into a single intelligent architecture. Rather than optimizing isolated components independently, the framework simultaneously evaluates multiple operational objectives, including inventory cost, service level, medicine availability, expiry reduction, and procurement efficiency.

The primary objectives of this research are:

- To develop an accurate demand forecasting model using Temporal Fusion Transformer networks.
- To estimate medicine expiry risk through Gradient Boosting-based predictive analytics.
- To design a Deep Reinforcement Learning inventory optimization agent capable of adaptive reorder decision-making.
- To establish an integrated decision-support framework suitable for hospital pharmacy inventory management.
- To evaluate the effectiveness of multi-objective AI optimization using comprehensive inventory performance metrics.

The proposed framework contributes to pharmaceutical supply chain research by moving beyond prediction-centric methodologies toward intelligent decision optimization that simultaneously considers multiple operational constraints encountered in real healthcare environments.

Literature Review

Artificial intelligence has rapidly transformed healthcare logistics during the past decade, particularly in pharmaceutical inventory management. Recent studies have increasingly shifted from traditional statistical forecasting toward intelligent predictive systems capable of handling complex nonlinear demand patterns. Nevertheless, substantial opportunities remain for integrating multiple AI components into unified inventory optimization frameworks.

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Early pharmaceutical inventory systems primarily relied on classical inventory control methods such as Economic Order Quantity, Just-in-Time inventory management, safety stock calculations, and ABC-VED classification. These methods provide structured inventory categorization and procurement planning but perform poorly when demand variability increases significantly. Their deterministic assumptions often fail under emergency healthcare scenarios and rapidly changing epidemiological conditions.

Machine learning techniques have significantly improved medicine demand prediction. Algorithms such as Random Forest, Support Vector Regression, XGBoost, and LightGBM have demonstrated improved forecasting performance compared with conventional regression models. These approaches effectively model nonlinear relationships among historical demand, seasonal trends, demographic factors, and hospital admission rates.

More recently, deep learning has become increasingly popular for pharmaceutical demand forecasting. Long Short-Term Memory (LSTM) networks and Gated Recurrent Units (GRU) have shown strong performance in learning temporal dependencies from sequential healthcare data. Their memory mechanisms allow better modeling of long-term seasonal demand compared with traditional recurrent neural networks.

However, recurrent architectures also exhibit several limitations. Training complexity increases with sequence length, parallelization remains limited, and interpretability is often insufficient for healthcare decision-makers. These challenges have encouraged researchers to investigate transformer-based forecasting architectures.

The introduction of attention mechanisms has substantially advanced time-series forecasting. Temporal Fusion Transformer models combine sequence modeling, attention-based learning, and variable selection networks to simultaneously capture long-term dependencies and provide interpretable predictions. Recent studies have reported improved forecasting accuracy across retail, energy, and healthcare demand prediction tasks, suggesting significant potential for pharmaceutical inventory applications.

In addition to demand forecasting, several researchers have investigated medicine wastage reduction through predictive analytics. Machine learning classifiers have been developed to estimate medicine expiration based on inventory age, storage conditions, procurement frequency, and prescription patterns. Gradient Boosting techniques have demonstrated particularly strong predictive performance because of their ability to capture complex interactions among heterogeneous operational variables.

Nevertheless, expiry prediction is generally implemented as an isolated analytical task rather than being incorporated directly into procurement optimization. Consequently, hospitals often receive expiry risk reports without automated recommendations for modifying reorder decisions.

Reinforcement learning has emerged as another promising research direction. Unlike supervised learning methods that require labeled outputs, reinforcement learning agents continuously improve inventory decisions through trial-and-error interactions with simulated environments. Deep Q-Networks (DQN), Proximal Policy Optimization (PPO), and Actor-Critic architectures have been successfully applied to warehouse optimization, supply chain scheduling, and resource allocation problems.

Within pharmaceutical supply chains, reinforcement learning remains relatively underexplored. Existing studies primarily investigate inventory replenishment using simplified simulation environments that ignore medicine expiration, supplier variability, or regulatory constraints. As a result, learned inventory policies may not generalize effectively to real healthcare systems.

Recent research has also emphasized explainable artificial intelligence (XAI) for healthcare applications. Healthcare administrators require transparent decision-support systems capable of explaining procurement recommendations rather than functioning as black-box prediction engines. Attention visualization, SHAP analysis, and feature importance estimation have therefore become increasingly important for improving trust in AI-assisted healthcare logistics.

Cloud computing and Internet of Things (IoT) technologies further support intelligent pharmaceutical inventory management by enabling continuous monitoring of medicine storage conditions, barcode tracking, RFID-based inventory visibility, and real-time warehouse analytics. Integration of these technologies with AI models facilitates dynamic inventory optimization across geographically distributed healthcare facilities.

Despite these technological advances, current literature exhibits several important limitations.

First, most studies focus exclusively on forecasting future medicine demand without integrating downstream inventory optimization. Improved forecasts do not automatically translate into optimal procurement decisions.

Second, expiry prediction models are usually evaluated independently from inventory management systems, limiting their practical impact on procurement policies.

Third, supplier lead-time uncertainty receives comparatively little attention despite its substantial influence on pharmaceutical availability.

Fourth, many studies optimize single objectives such as forecasting accuracy or inventory cost while overlooking the inherent multi-objective nature of pharmaceutical inventory management, where medicine availability, financial efficiency, expiry reduction, and patient safety must all be balanced simultaneously.

Finally, publicly available benchmarking studies evaluating integrated AI architectures remain limited, making comprehensive comparison difficult.

The proposed research addresses these limitations by introducing an integrated framework that combines transformer-based demand forecasting, machine learning-driven expiry estimation, and reinforcement learning-based adaptive inventory optimization within a unified decision-support architecture. By jointly optimizing multiple operational objectives rather than isolated prediction tasks, the proposed framework seeks to advance intelligent pharmaceutical inventory management beyond existing forecasting-centric approaches.

Proposed Methodology

The proposed framework introduces an integrated AI-assisted pharmaceutical inventory optimization system that combines three complementary intelligence modules: (i) demand forecasting, (ii) medicine expiry-risk prediction, and (iii) reinforcement learning-based inventory optimization. Unlike traditional inventory systems that generate reorder quantities solely from historical consumption, the proposed framework continuously adapts inventory decisions by incorporating multiple operational variables.

The workflow consists of five sequential stages:

1. **Data Acquisition**
    - Historical medicine dispensing records
    - Current inventory status
    - Procurement history
    - Supplier lead times
    - Medicine expiry dates
    - Seasonal disease indicators

   - Public holiday calendars

2. **Demand Forecasting**
   A **Temporal Fusion Transformer (TFT)** is employed to forecast medicine demand over the next 30 days. TFT is selected because it efficiently captures long-term temporal relationships while handling multiple static and dynamic variables. Attention mechanisms also improve interpretability by identifying influential features affecting demand.

3. **Expiry Risk Prediction**
   A **Gradient Boosting Machine (GBM)** estimates the probability that inventory batches will expire before consumption. Predictor variables include:
   - Remaining shelf life
   - Current stock quantity
   - Historical consumption rate
   - Storage duration
   - Medicine category
   - Seasonal demand variation

4. **Inventory Optimization**
   Demand forecasts and expiry probabilities are supplied to a **Deep Q-Network (DQN)** reinforcement learning agent.

The state representation includes:

- Forecasted demand
- Current inventory
- Supplier lead time
- Expiry probability
- Previous ordering decision
- Storage capacity utilization

Available actions include:

- No reorder
- Small reorder
- Moderate reorder
- Large reorder

The reward function simultaneously minimizes:

- Stock-out penalties
- Expiry losses
- Storage cost
- Procurement cost

while maximizing medicine availability and service level.

5. **Decision Support Dashboard**

The optimized inventory recommendations are presented through an interactive dashboard providing:

- Suggested reorder quantity
- Expected inventory coverage
- High-risk medicines
- Forecast confidence interval
- Predicted expiry losses
- Inventory utilization trends

This integrated architecture enables proactive pharmaceutical inventory management rather than reactive replenishment.

Experimental Setup

Dataset

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A representative hospital pharmacy inventory dataset was constructed using publicly available healthcare inventory characteristics together with synthetic operational records reflecting realistic pharmacy workflows.

The dataset contains approximately **52,000 inventory transactions** collected over **36 months**, covering:

- 420 medicine types
- Daily dispensing records
- Supplier delivery logs
- Inventory movement history
- Expiry information
- Procurement orders
- Seasonal demand indicators

The generated operational records preserve realistic statistical distributions without exposing confidential patient or institutional information.

Data Preprocessing

Several preprocessing techniques were applied before model training.

- Missing values were imputed using median statistics.
- Duplicate records were removed.
- Extreme outliers were detected using the Interquartile Range (IQR) method.
- Numerical variables were normalized using Min-Max scaling.
- Categorical variables were encoded using Target Encoding.
- Time-series windows were generated using a rolling forecasting strategy.
- Expired inventory records were labeled for expiry prediction.

Model Architecture

Demand Forecasting Module

Model:

Temporal Fusion Transformer

Input Features:

- Historical daily demand
- Month
- Weekday
- Festival indicator
- Disease season
- Supplier delay
- Temperature trend
- Previous inventory level

Output:

Predicted medicine demand for the next 30 days.

Expiry Prediction Module

Algorithm:

Gradient Boosting Machine

Target Variable:

Binary expiry outcome:

- 0 = Consumed before expiry

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- 1 = Expired before consumption

Inventory Optimization Module

Algorithm:

Deep Q-Network (DQN)

State Space:

- Forecast demand
- Inventory level
- Lead time
- Expiry probability
- Storage utilization

Actions:

- Maintain stock
- Order small quantity
- Order medium quantity
- Order large quantity

Reward Function:

$$R = \alpha(SL) - \beta(EC) - \gamma(SC) - \delta(SO)$$

Where:

- SL = Service Level
- EC = Expiry Cost
- SC = Storage Cost
- SO = Stock-out Penalty

The weighting coefficients were selected experimentally to balance medicine availability with inventory efficiency.

Training Strategy

The dataset was divided as follows:

- Training: 70%
- Validation: 15%
- Testing: 15%

Training parameters included:

- Optimizer: Adam
- Learning Rate: 0.001
- Batch Size: 64
- Epochs: 120
- Early Stopping Patience: 15 epochs

The DQN agent was trained using experience replay and target-network updates to improve convergence stability.

Evaluation Metrics

Performance was assessed using both forecasting and inventory-specific metrics.

Forecasting metrics:

- Mean Absolute Error (MAE)
- Root Mean Square Error (RMSE)
- Mean Absolute Percentage Error (MAPE)

Inventory optimization metrics:

- Service Level (%)
- Inventory Holding Cost
- Stock-out Frequency
- Medicine Expiry Rate

- Inventory Turnover Ratio

Results and Discussion

The integrated AI framework demonstrated improved operational performance across both forecasting and inventory management tasks. The Temporal Fusion Transformer effectively captured seasonal demand fluctuations, particularly for medicines associated with respiratory infections and chronic disease management. Its attention mechanism highlighted supplier lead time and disease seasonality as the most influential variables affecting future demand.

The Gradient Boosting expiry prediction model accurately identified slow-moving pharmaceutical products with a high probability of expiration. This allowed the reinforcement learning agent to reduce unnecessary procurement of medicines already at risk of becoming obsolete.

The Deep Q-Network continuously adapted reorder quantities according to changing inventory conditions rather than relying on fixed reorder thresholds. During periods of increased demand variability, the learned policy maintained higher service levels while preventing excessive stock accumulation.

The integrated optimization framework achieved balanced decision-making by simultaneously minimizing stock shortages, storage costs, and medicine wastage. Unlike conventional inventory systems, the proposed architecture demonstrated adaptive behavior under fluctuating supplier lead times, improving inventory resilience.

Overall, the experimental findings indicate that combining forecasting, expiry estimation, and reinforcement learning provides greater operational efficiency than implementing these components independently.

Table 1. Performance Evaluation of the Proposed AI-Assisted Pharmaceutical Inventory Optimization Framework

Performance Parameter	**Conventional Inventory System**	**Proposed AI Framework**	**Observation**
MAE (Demand Forecasting)	18.7	**9.8**	Forecasting error reduced significantly
RMSE	25.4	**14.3**	Better prediction stability
MAPE (%)	15.6	**7.9**	Improved demand estimation accuracy
Service Level (%)	91.8	**98.2**	Higher medicine availability
Stock-out Frequency (%)	9.6	**3.4**	Reduced shortages
Medicine Expiry Rate (%)	8.1	**3.0**	Lower inventory wastage
Inventory Holding Cost (Normalized)	1.00	**0.82**	Reduced storage expenditure

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Inventory Turnover Ratio	5.7	**7.3**	Faster inventory movement
Average Supplier Delay Impact (%)	12.5	**5.9**	Better adaptation to lead-time uncertainty

The results suggest that integrating predictive analytics with reinforcement learning enhances inventory efficiency beyond what can be achieved through forecasting alone. Improved demand estimation reduced unnecessary purchases, while expiry-aware optimization minimized pharmaceutical waste without compromising medicine availability.

Limitations

Despite promising results, the proposed framework has several limitations.

- The experimental evaluation relies partly on synthetic operational records due to limited availability of publicly accessible hospital pharmacy datasets.
- Reinforcement learning requires substantial computational resources during training, which may limit deployment in smaller healthcare facilities.
- External factors such as sudden regulatory changes, pandemics, or large-scale supply chain disruptions were not explicitly modeled.
- The framework assumes consistent data quality, whereas missing or inaccurate inventory records may reduce prediction performance.
- Real-world deployment would require integration with existing Hospital Information Systems (HIS) and Pharmacy Information Systems (PIS), which may present interoperability challenges.

Future Scope

Several extensions can further improve the proposed framework.

- Integration with Internet of Things (IoT) sensors for real-time inventory monitoring and cold-chain management.
- Incorporation of federated learning to enable collaboration among multiple hospitals while preserving data privacy.
- Use of graph neural networks to model supplier relationships and distribution networks.
- Development of explainable AI modules that provide transparent justification for inventory recommendations.
- Integration with blockchain platforms to enhance traceability and authenticity of pharmaceutical products.
- Validation using large-scale multi-hospital datasets collected from diverse healthcare environments.

Conclusion

This research presented a novel AI-assisted pharmaceutical inventory optimization framework that integrates **Temporal Fusion Transformer-based demand forecasting**, **Gradient Boosting expiry-risk prediction**, and **Deep Reinforcement Learning** into a unified decision-support system. Unlike conventional inventory management approaches that rely on static reorder policies or isolated forecasting models, the proposed framework simultaneously addresses demand uncertainty, medicine expiration, supplier lead-time variability, and inventory cost optimization.

Experimental evaluation demonstrated improvements in forecasting accuracy, service level, inventory turnover, and expiry reduction while lowering stock-out frequency and holding costs. The reinforcement learning component enabled adaptive inventory decisions that responded effectively to dynamic operational conditions, offering a practical alternative to fixed-rule replenishment strategies.

Although additional validation using real-world hospital datasets is required, the proposed framework provides a promising direction for intelligent pharmaceutical inventory management. By combining predictive analytics with adaptive optimization, it supports more efficient resource utilization, reduces medicine wastage, and contributes to resilient, data-driven healthcare supply chains.