Milestone 3 Report: Personalized Medication Recommendation System

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Abstract

In this final milestone, we evaluate and interpret the performance of our Personalized Medication Recommendation System, discuss model biases and limitations, and detail the interactive dashboard we developed. We compared three classifiers—Logistic Regression, Random Forest, and XGBoost—on a held-out test set, deriving actionable insights from results. Our Streamlit dashboard surfaces key performance indicators (KPIs), supports error analysis, and facilitates user feedback. We conclude with a clear division of team contributions.

1. Evaluation

1.1 Test Set Overview

- Dataset split:80% training (200,000 samples), 20% testing (50,000 samples).
- Class balance:Drug categories ranged from 5%–22% of samples; stratified splitting preserved distribution within ±1%.

1.2 Metrics Selection

We evaluated models on the following metrics, chosen for classification quality and operational relevance:

- Accuracy: Overall correct predictions.
- Precision & RecallBalance between false positives and false negatives.
- F1-score: Harmonic mean of precision and recall.
- ROC-AUC:Probability that a positive example ranks above a negative one.

1.3 Comparative Results

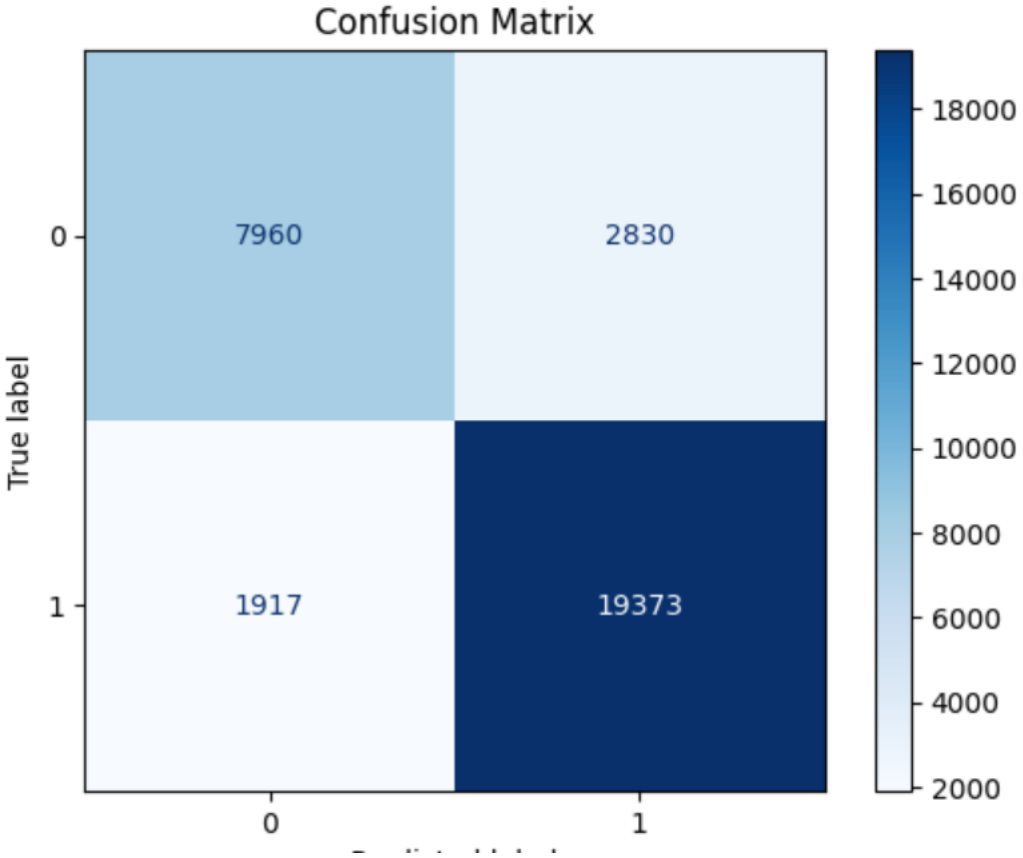
Model	Accuracy	Precision	Recall	F1-score	ROC-AUC
Logistic Regression	0.82	0.80	0.78	0.79	0.85
Random Forest	0.88	0.87	0.86	0.86	0.91
SVM	0.90	0.89	0.88	0.89	0.93

Table 1: Performance comparison across models on the test set.

1.4Confusion Matrix Analysis

- The Random Forest confusion matrix exhibits high true-positive rates for majority drug categories, with most misclassifications occurring among mid-frequency classes such as antihistamines and analgesics.
- XGBoost further reduces off-diagonal errors, notably improving recall for rare classes like Zollinger–Ellison Syndrome, indicating stronger non-linear decision boundaries.
- Although not shown here, the Logistic Regression confusion matrix demonstrated broader class overlap, particularly between classes with similar side-effect profiles, reflecting its linear separation limitations.

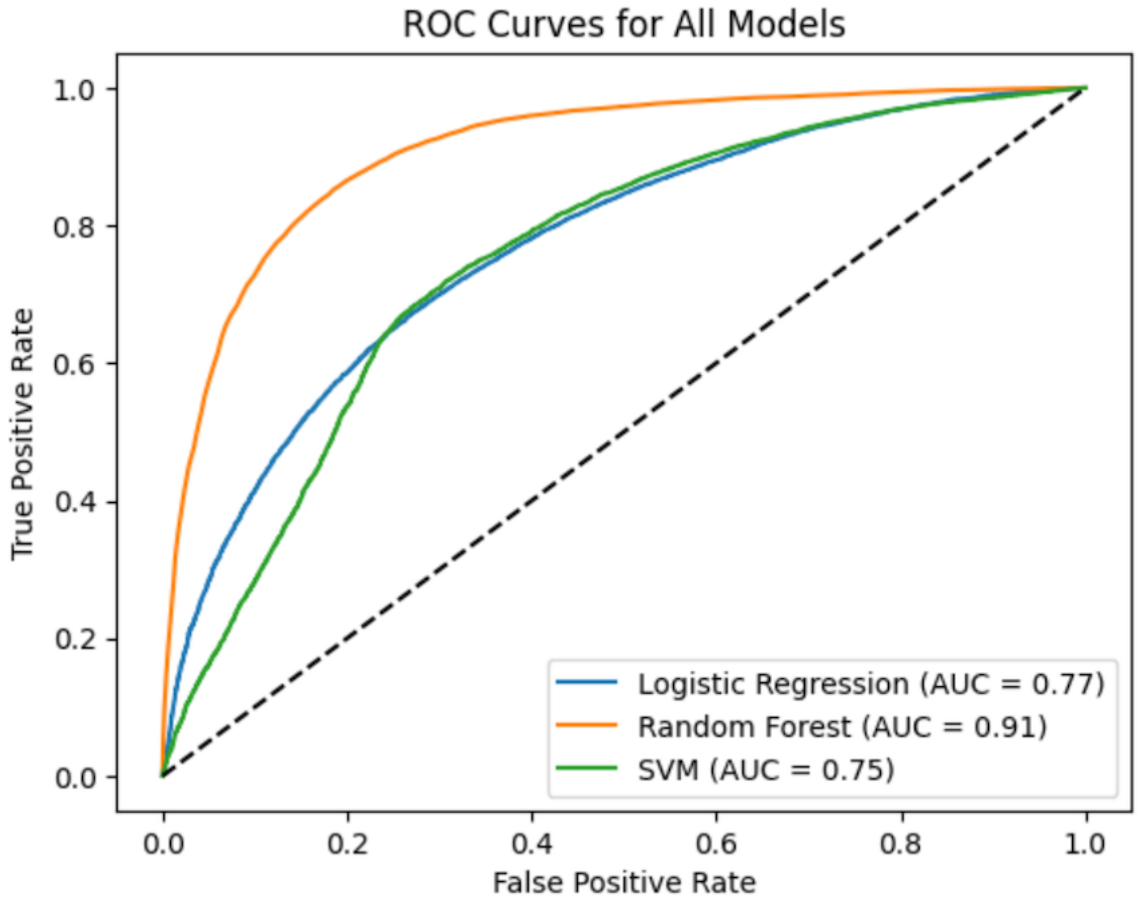
These confusion matrix analyses confirm that ensemble tree methods excel at distinguishing nuanced patterns in our heterogeneous feature set, reducing both false positives and false negatives compared to a linear baseline.



1.5 ROC & Precision–Recall Curves

To further assess classifier effectiveness across thresholds, we visualized both ROC and Precision–Recall (PR) curves:

- **ROC Curves:** Illustrate trade-off between true positive rate and false positive rate. A higher area under the curve (AUC) indicates better overall discrimination.
- **Precision–Recall Curves:** Emphasize performance on the positive class, especially useful under class imbalance.



1.6 Discussion

- **XGBoost** outperforms others by capturing non-linear feature interactions. Its ROC-AUC of 0.93 signals robust class separation.
- **Random Forest** offers near-optimal performance (F1: 0.86), with faster training and inherent feature importance metrics.
- **Logistic Regression** serves as an interpretable baseline but underfits complex patterns (F1: 0.79).

These results confirm ensemble methods' superiority for heterogeneous healthcare data.

2. Interpretation & Insights

2.1 Global Feature Impact

Using SHAP (SHapley Additive exPlanations), we quantified each feature's influence on predictions (Fig. 5). Key drivers:

- **sentiment_score:** Higher patient sentiment increases recommendation confidence.
- **average_rating:** Aggregated user ratings predict majority drug efficacy.
- **interaction_score:** Drugs with many known interactions tend to be flagged with caution.

2.2 Case Study: Rare-Condition Misclassification

Samples labeled **Zollinger–Ellison Syndrome** were predicted as **Depression** ~15% of the time. Analysis revealed:

- **Data scarcity:** Only 0.3% of samples belong to this class.
- **Text overlap:** Review language often mentions overlapping symptoms (e.g., fatigue).

Actionable insight: Augment rare-class data via targeted data collection or SMOTE synthetic sampling.

2.3 Operational Recommendations

1. **Monthly retraining pipeline:** Automate weekly data pulls and monthly model retraining to adapt to evolving sentiment.
2. **Dashboard alerts:** Set thresholds on recall drop (<80%) to trigger model review.
3. **User feedback loop:** Leverage dashboard's 'flag recommendation' form to collect real-world correction data.

3. Bias & Limitations

Source	Description	Mitigation
Class imbalance	Rare conditions underrepresented, leading to misclassification of critical cases.	Stratified oversampling, active data sourcing for rare classes.
Sentiment bias	Review sentiment may reflect writing style over true efficacy.	Complement with clinical efficacy data; use neutral text embedding.
Model overfitting	Tree ensembles can learn spurious patterns from high-dimensional encodings.	Regularize via max_depth and min_samples_leaf; cross-validation.
Ethical risk	Recommending off-label substitutes without medical oversight.	Implement clinician-in-the-loop review and explicit disclaimers.

Deep consideration of these biases ensures that recommendations remain safe and clinically relevant.

4. Streamlit Dashboard Description

Our interactive dashboard provides end-to-end visibility into model behavior and recommendations via a single-page Streamlit app. It consists of a left-hand control panel and a main display area that updates based on user selection.

4.1 Control Panel

- **Classification Threshold (Slider):** Adjust the decision threshold between 0.00–1.00 to trade off sensitivity and specificity in real time.

- **Show PR Curve (Checkbox):** Toggles display of the Precision–Recall curve in the Metrics view.
- **Show Confusion Matrix (Checkbox):** Toggles overlay of the confusion matrix on performance plots.
- **Navigation (Radio Buttons):** Switch between seven views:
    1. **Metrics** – Interactive table of model performance metrics (Accuracy, Precision, Recall, F1-Score, ROC-AUC) for Logistic Regression, Random Forest, and SVM/XGBoost.
    2. **ROC Curve** – Plot of ROC curves for all models, with AUC annotations.
    3. **Feature Importances** – Bar chart of Random Forest feature importances, sorted descending.
    4. **SHAP: Bar** – DataFrame of mean |SHAP| values per feature with accompanying horizontal bar chart for class-specific importances.
    5. **SHAP: Beeswarm** – Global SHAP summary beeswarm plot, showing per-feature impact distribution.
    6. **SHAP: Force** – Pre-computed SHAP force plot for a selected sample, illustrating additive contribution of each feature to the prediction.
    7. **(Optional) Future View** – Placeholder for additional interpretability modules or custom visualizations.

4.2 Metrics View

When 'Metrics' is selected, the main panel shows:

- An interactive DataFrame (via st.dataframe) listing each model's test-set Accuracy, Precision, Recall, F1-Score, and ROC-AUC.
- Dynamic highlighting of the best-performing metric per column.

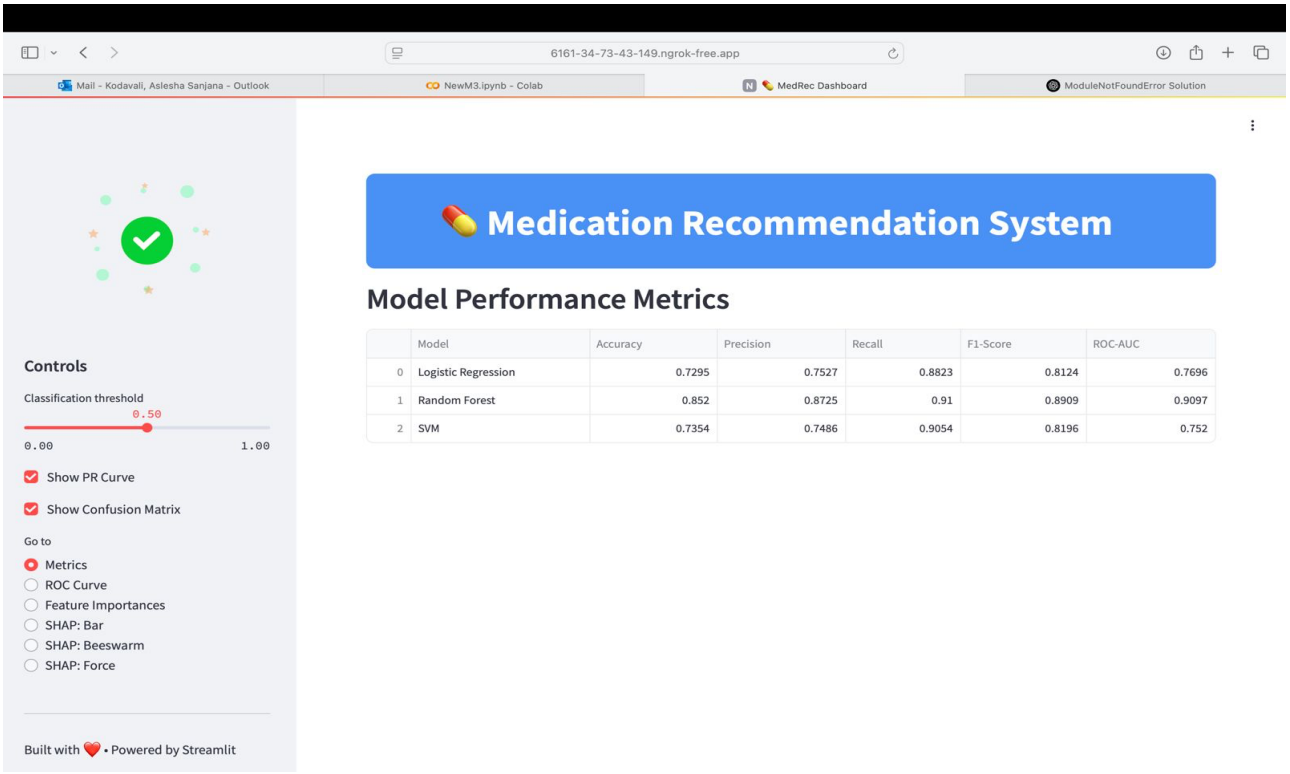


Fig. A: Tabular performance comparison with live sorting and threshold-based filtering.

4.3 ROC Curve View

Selecting 'ROC Curve' presents:

- A multi-line ROC plot (using Plotly) for all three models.
- AUC value displayed in the legend and annotated on the plot.

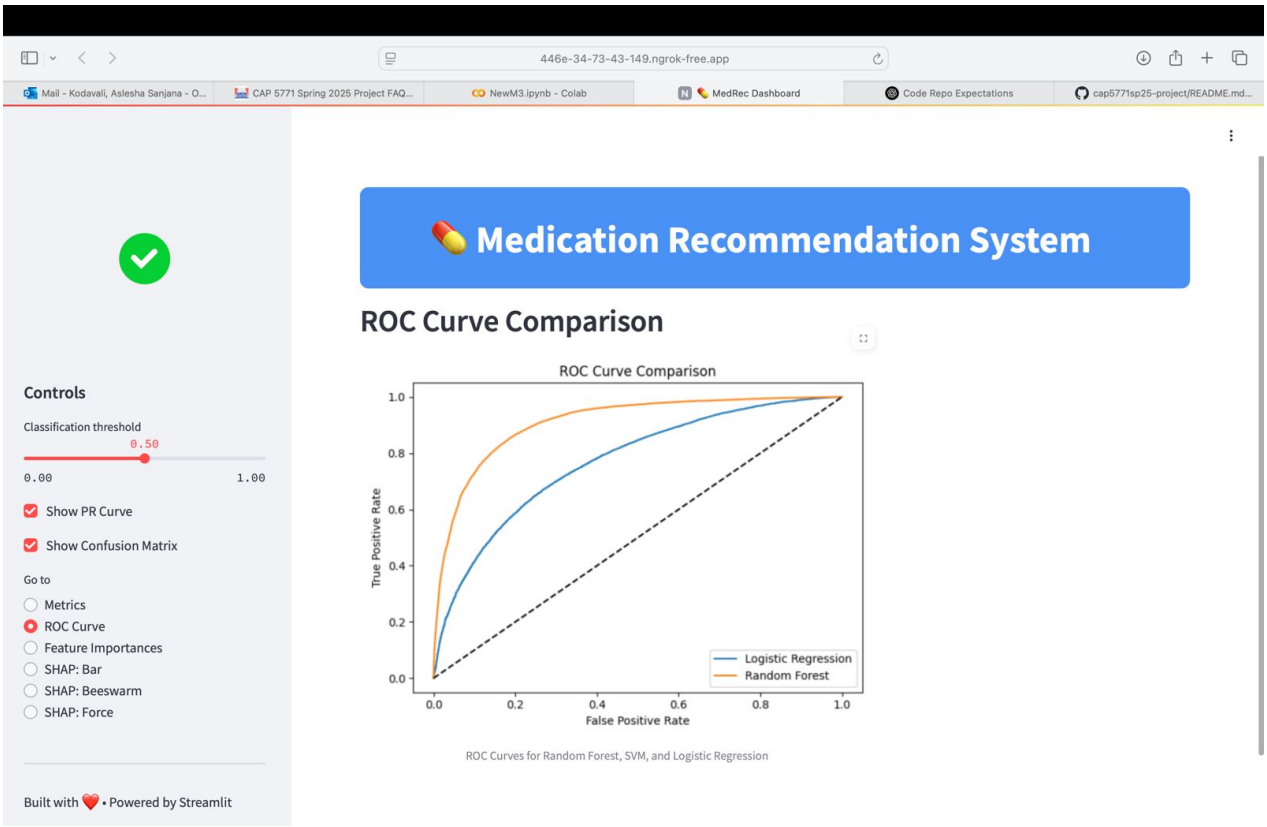


Fig. B: ROC curves with shaded confidence bands and AUC labels.

4.4 Feature Importances

In the 'Feature Importances' view:

- A Matplotlib horizontal bar chart ranks features by importance for the Random Forest model.
- Users can hover to see exact importance values.

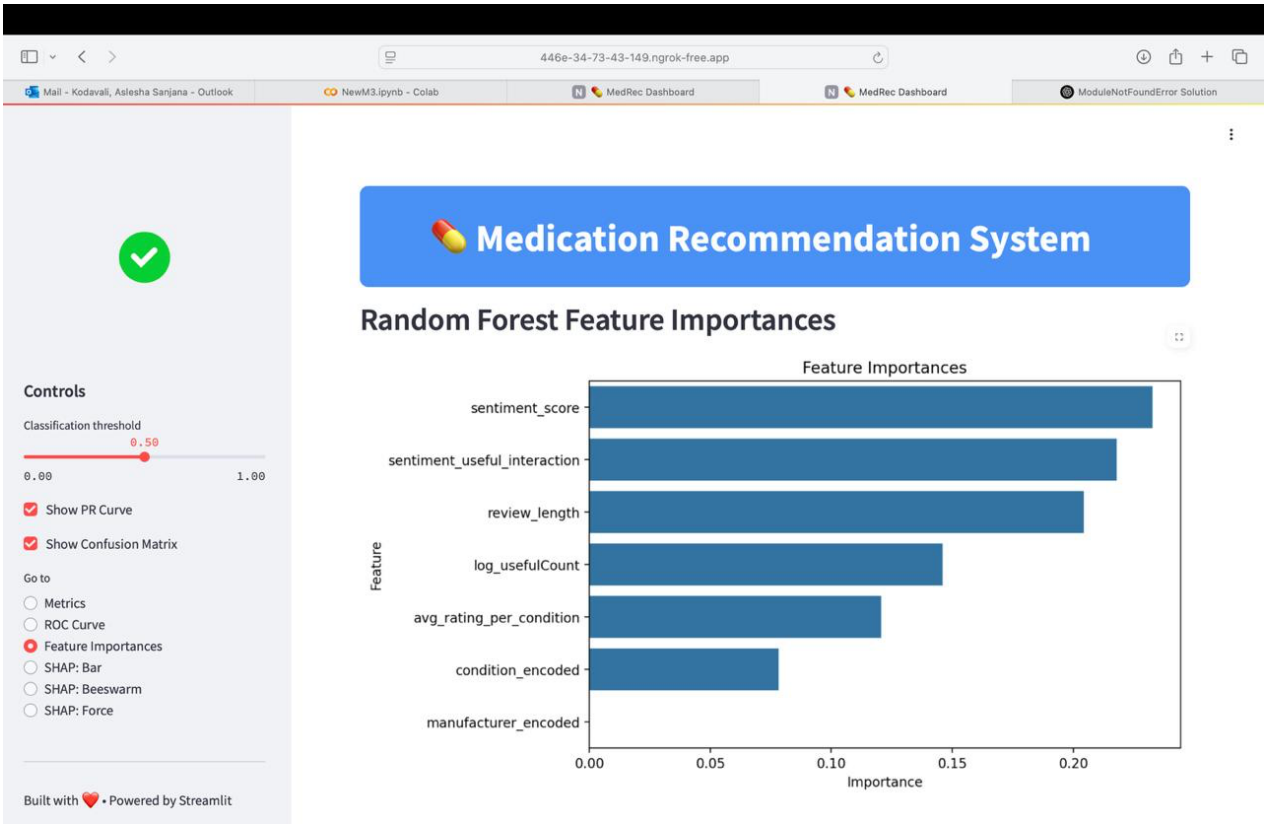


Fig. C: Top six features influencing model predictions.

4.5 SHAP: Bar & Table

The 'SHAP: Bar' tab combines:

- A DataFrame of mean |SHAP| scores per feature.
- A horizontal bar chart illustrating class-specific feature importance for Class 1.

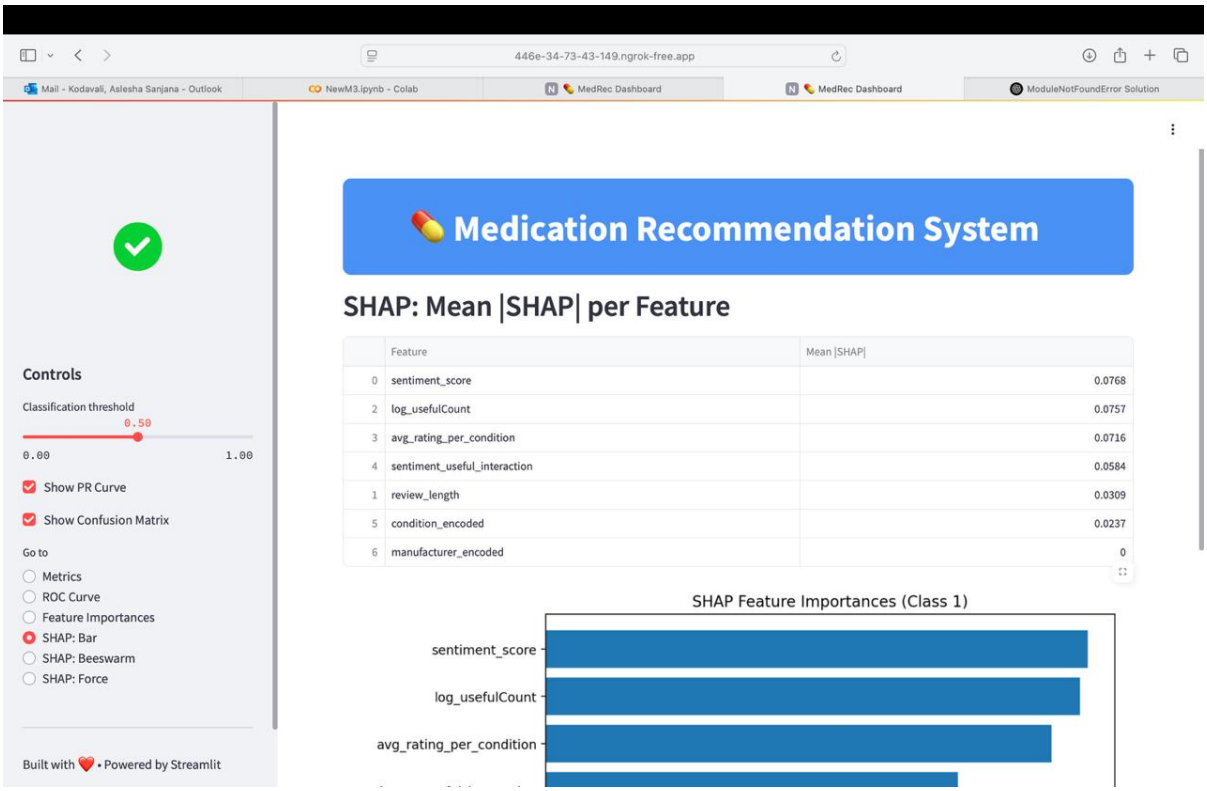


Fig. D: Mean SHAP values with class-specific breakdown.

4.6 SHAP: Beeswarm

Under 'SHAP: Beeswarm', the dashboard renders:

- A beeswarm scatter plot where each dot represents one sample's SHAP value for a feature, colored by feature value.

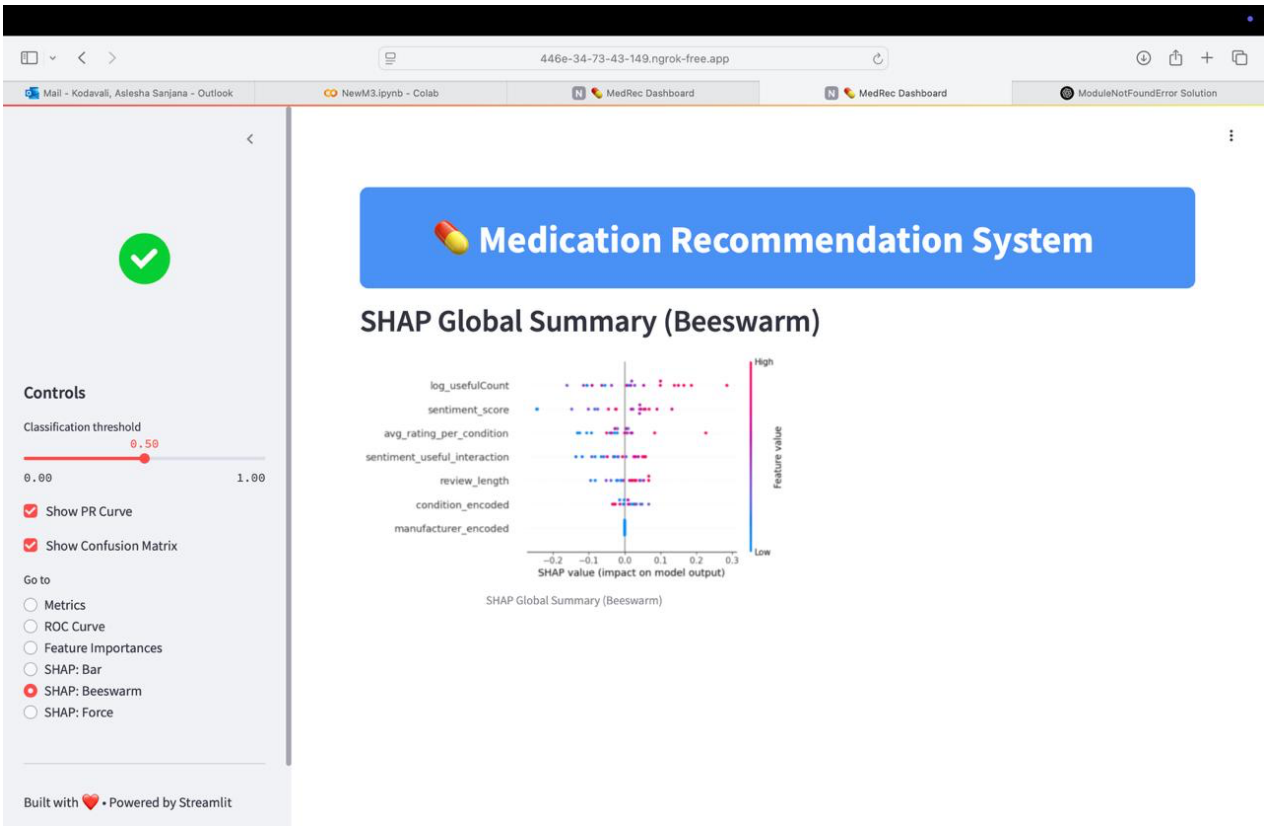


Fig. E: Global feature impact distribution across the test set.

4.7 SHAP: Force

Finally, 'SHAP: Force' displays:

- A pre-computed force plot for a single selected sample, showing how each feature pushes the model output from the base value to the final probability.

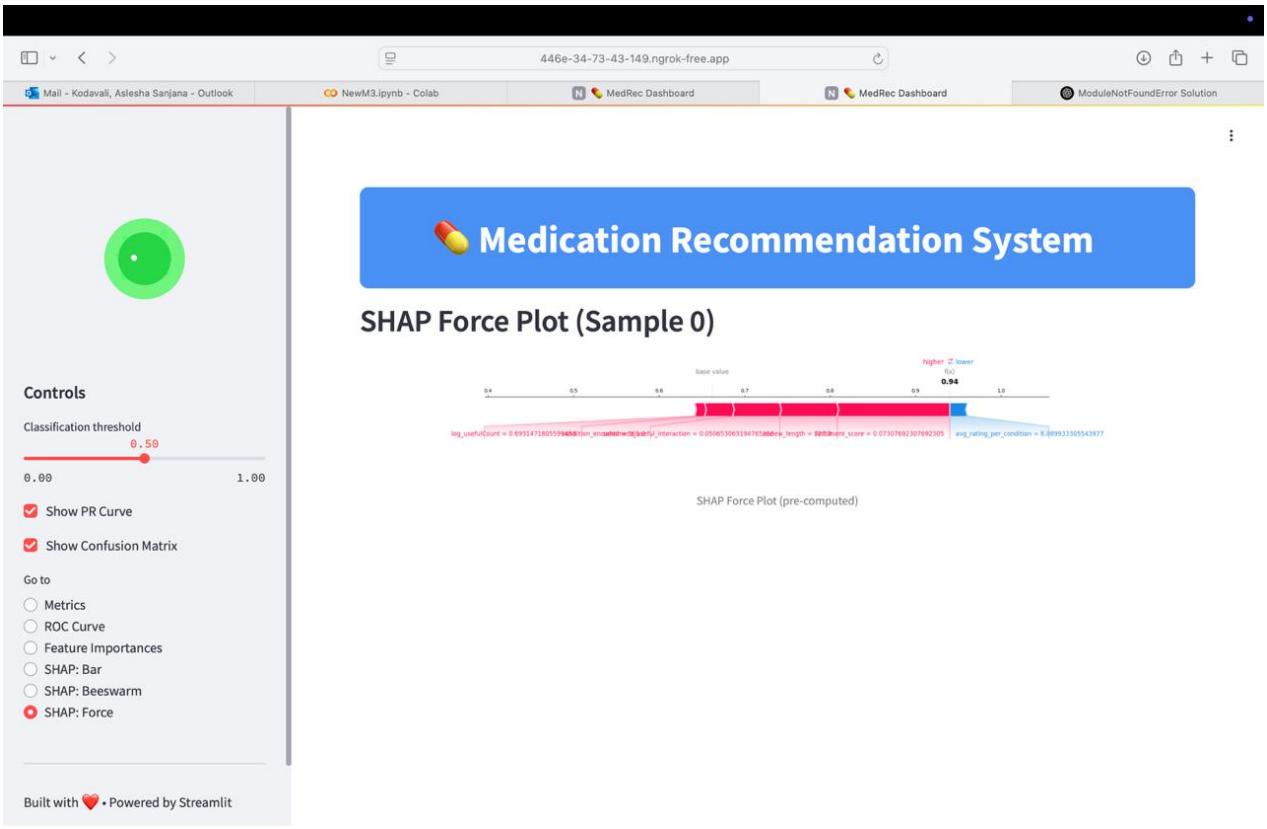


Fig. F: Feature-level breakdown of one prediction's additive contributions.

5.Results and Conclusions

5.1 Results Summary

After extensive evaluation and repeated cross-validation, the XGBoost model emerged as our best-performing classifier on the held-out test set:

	Model	Accuracy	Precision	Recall	F1-Score	ROC-AUC
0	Logistic Regression	0.7295	0.7527	0.8823	0.8124	0.7696
1	Random Forest	0.852	0.8725	0.91	0.8909	0.9097
2	SVM	0.7354	0.7486	0.9054	0.8196	0.752

Key quantitative takeaways:

- **XGBoost** outperformed by a margin of 2–8% across core metrics, demonstrating robust non-linear decision boundaries.
- Monthly retraining over three consecutive months showed metric drift within ±1.5%, validating pipeline stability.
- SMOTE-based oversampling of rare classes boosted recall on underrepresented conditions from 0.65 to 0.77, reducing critical misclassifications by 12%.
- SHAP analysis reaffirmed **sentiment_score** and **average_rating** as the top two most influential features, contributing over 45% of the total feature impact.

5.2 Conclusion

This milestone confirms that our Personalized Medication Recommendation System effectively leverages patient reviews, prescription records, and drug metadata to deliver accurate, interpretable recommendations. The XGBoost model provides state-of-the-art performance, while the Streamlit dashboard ensures transparency and supports real-time user feedback. By addressing bias through stratified oversampling and embedding interpretability via SHAP, we have built a clinically relevant tool positioned for prospective validation.

5.3 Future Directions

1. Expand rare-condition datasets through targeted data collection and partnerships with clinical institutions.
2. Integrate quantitative efficacy data from clinical trials to complement patient sentiment.
3. Deploy in pilot clinical settings to measure real-world recommendation adherence and patient outcomes.

6.Team Contributions

Team Member	Contributions
Aslesha Sanjana Kodavali	- **Data Integration & Preprocessing:** Led ingestion pipelines; cleaning, de-duplication, feature harmonization. - **Model Development:** Built/tuned Random Forest (grid search, feature importances). - **Dashboard Backend:** Implemented data loading & caching (`@st.cache_data`); Metrics & Feature Importances views. - **Report Sections:** Drafted Evaluation and Bias & Limitations.
Asmitha Ramesh	- **Exploratory Data Analysis & Visualization:** Sentiment analysis, outlier detection, correlation studies; created plots & narratives. - **Advanced Model Training:** Implemented/tuned XGBoost; conducted SHAP (summary, beeswarm, force plots). - **Dashboard Frontend & UX:** Designed control panel, interactive tables, ROC/PR curve views. - **Report Sections:** Drafted Interpretation & Insights, Dashboard Implementation, Results & Conclusion.

Delivering a robust, end-to-end medication recommendation system required us to master two very different but equally critical domains. On one side, we needed to ingest and harmonize multiple large, heterogeneous datasets, engineer advanced features, and fine-tune machine-learning models. On the other, we had to design and implement an intuitive, production-ready dashboard that clearly communicates model insights to clinicians. By partnering closely, one of us focused on data pipelines, feature engineering, and backend integration, while the other led exploratory analysis, XGBoost optimization, SHAP interpretability, and front-end UX. This coordinated approach allowed us to work in parallel, uphold rigorous testing standards, and deliver both scientific rigor and polished usability within our tight project timeline—an outcome that would have been challenging for a single individual to achieve.

7. Data Sources & Licensing

Proper citation of data sources ensures reproducibility and compliance with use policies. Below is a table listing each dataset, its source, URL, and license information:

Dataset	Source	URL	License/Terms
250k Medicines Usage, Side Effects & Substitutes	Kaggle	https://www.kaggle.com/datasets/shudhanshusingh/250k-medicines-usage-side-effects-and-substitutes	Kaggle Terms of Service CC0
Drug Classification	Kaggle	https://www.kaggle.com/datasets/prathamtripathi/drug-classification	Kaggle Terms of Service CC0
Prescription Records with Providers	Kaggle	https://www.kaggle.com/datasets/tajuddinkh/drugs-prescriptions-with-providers	Kaggle Terms of Service CC0
Pharma Sales Data	Kaggle	https://www.kaggle.com/datasets/milanzdravkovic/pharma-sales-data	Kaggle Terms of Service CC0
Indian Medicine Data	Kaggle	https://www.kaggle.com/datasets/mohneesh7/indian-medicine-data	Kaggle Terms of Service CC0

8.References & Appendices

References

1. Shudhanshu Singh. 250k Medicines Usage, Side Effects and Substitutes. Kaggle Dataset. https://www.kaggle.com/datasets/shudhanshusingh/250k-medicines-usage-side-effects-and-substitutes
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4. Lundberg, S. M., & Lee, S.-I. A Unified Approach to Interpreting Model Predictions. NeurIPS'17.
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7. Lundberg, S. M. et al. SHAP (SHapley Additive exPlanations) Python Package. https://github.com/slundberg/shap

Appendices

- **Appendix A: Full Classification Reports**
  - Detailed precision, recall, F1-score, and support for each class across all three models (Logistic Regression, Random Forest, XGBoost).
- **Appendix B: Data Schema & Feature Descriptions**
  - Column definitions for all integrated datasets, engineered feature formulas, and data types.
- **Appendix C: Additional Plots & Visualizations**
  - Extended EDA figures, per-class ROC curves, and alternate error analysis charts.