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Course Title: Data Analytics Services (BUAN305)

DATA ANALYTICS SERVICES REPORT

Project Title: Drug Response Prediction for Typhoid Fever

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1. Introduction

a. Background of the Study

Typhoid fever is a life-threatening infection caused by the bacterium *Salmonella Typhi*. It remains prevalent in many developing countries, resulting in significant morbidity and mortality. Early diagnosis and the administration of appropriate antibiotic treatment are critical for patient recovery. However, due to increasing antibiotic resistance, identifying the most effective treatment for a patient has become increasingly challenging.

Traditional methods of prescribing antibiotics rely heavily on clinical judgment and bacterial culture tests, which can be time-consuming. Artificial Intelligence (AI) has the potential to revolutionize this process by analyzing patient data to predict the likely success of different treatments, leading to faster and more accurate decisions. This project explores the application of machine learning models to predict the efficacy of drug treatments for Typhoid Fever patients based on their clinical profiles.

b. Relevance of the Project in AI

The integration of AI in healthcare, particularly in predictive modeling, is an emerging trend that has demonstrated substantial benefits. AI techniques such as machine learning can analyze complex datasets, recognize patterns, and make predictions that support clinical decision-making. This project contributes to the field by developing a predictive model tailored to infectious diseases, specifically Typhoid Fever. The system not only predicts drug efficacy but also emphasizes model explainability to ensure that clinicians can understand and trust the AI's recommendations.

c. Scope of the project

The scope of the project includes:

- Developing predictive models using clinical data of Typhoid Fever patients.
- Evaluating the models' performance using various statistical metrics.
- Designing a prototype tool that provides drug efficacy predictions for healthcare professionals.

The project focuses solely on Typhoid Fever patients and assumes that the data provided is accurate and representative of real-world conditions.

d. Significance of the Work

This work is significant for several reasons:

- It provides a framework for personalized medicine in infectious diseases.
- It reduces dependency on empirical prescribing and bacterial culture wait times.
- It contributes to the global fight against antibiotic resistance by promoting more targeted treatment strategies.
- It demonstrates a practical application of machine learning and explainable AI in healthcare, setting the stage for future expansions to other diseases.

2. Objectives of the Project

a. Aims and Objectives

The primary aim of this project is to develop an AI-driven solution to predict the efficacy of drug treatments for Typhoid Fever patients. The specific objectives include:

- **Objective 1**: To preprocess and clean patient datasets to ensure high-quality input for modeling.
- **Objective 2**: To apply and evaluate different machine learning algorithms for predictive accuracy.
- **Objective 3**: To interpret the model outputs using explainable AI techniques for transparency.
- **Objective 4**: To deploy a prototype clinical tool that integrates predictions into hospital systems.

3. Literature Review

The application of artificial intelligence (AI) and machine learning (ML) in healthcare, particularly for drug efficacy prediction, has grown rapidly over the past decade. Early work by Gottlieb et al. (2011) introduced computational frameworks for drug repositioning by analyzing genomic and chemical properties of drugs, highlighting the potential of ML models in uncovering hidden therapeutic associations. Following this, Alaa and van der Schaar (2018) proposed a Bayesian framework for individualized treatment effect prediction, emphasizing the need for patient-specific modeling to better understand drug responses across diverse populations.

Deep learning techniques have also played a major role in advancing healthcare predictions. Esteva et al. (2019) demonstrated the effectiveness of convolutional neural networks (CNNs) and recurrent neural networks (RNNs) in clinical diagnosis tasks, establishing a foundation for leveraging large-scale patient datasets to enhance predictive accuracy. However, as Ching et al. (2018) pointed out, healthcare data often suffer from challenges such as missing values, high dimensionality, and label noise, which complicate the direct application of deep learning models. These challenges necessitate careful preprocessing, model selection, and validation, all of which are critical components in the design of effective clinical decision-support systems.

Another important dimension of AI in healthcare is model interpretability. Doshi-Velez and Kim (2017) emphasized that interpretability is not merely desirable but essential for machine learning models deployed in clinical settings. Without explainability, clinicians may be hesitant to trust or act upon model recommendations. Holzinger et al. (2017) further discussed the concept of interactive machine learning, where systems are designed to foster collaboration between human experts and AI models, thereby improving trust, transparency, and ultimately clinical outcomes.

Recent studies have also addressed the importance of explainable AI (XAI) tools in the healthcare domain. Lundberg and Lee (2017) introduced SHAP values as a unified approach to interpreting model predictions, enabling practitioners to understand the contribution of each feature toward the final prediction. Similarly, Ribeiro et al. (2016) proposed the LIME framework, which provides local explanations for individual model predictions, making black-box models more accessible to healthcare professionals.

In terms of machine learning algorithms, Random Forests (RF) have emerged as particularly effective for healthcare predictions due to their robustness, interpretability, and ability to handle non-linear

relationships (Breiman, 2001). Random Forests combine multiple decision trees to reduce overfitting and improve generalization, making them well-suited for datasets with noisy or missing data, a common challenge in clinical environments. Studies such as Couronné et al. (2018) have shown that Random Forest models consistently outperform traditional regression and logistic regression models in clinical risk prediction tasks, further validating their relevance to healthcare AI systems.

Specifically regarding infectious diseases, machine learning applications in predicting outcomes and treatment responses have gained traction. For example, a study by Attai et al. (2022) demonstrated the utility of machine learning models, including Random Forests, to predict antimicrobial resistance patterns in Typhoid Fever based on patient demographics and clinical features. Their findings highlighted that machine learning could guide clinicians in selecting effective treatments and minimizing resistance risks, a goal closely aligned with the objectives of our project.

Furthermore, research by Chiu et al. (2021) emphasized the potential of ML models to predict bacterial infection outcomes and optimize antibiotic therapies. Although not exclusively focused on typhoid, their approach is directly applicable, as it combines patient-level data with ensemble learning techniques to improve drug efficacy predictions.

Despite these advancements, significant gaps remain. Few models have been developed specifically for predicting drug efficacy for Typhoid Fever or similar infectious diseases prevalent in lower- and middle-income countries. Additionally, while substantial progress has been made in developing accurate models, the integration of explainability and user trust mechanisms into clinical workflows remains limited. Our project directly addresses these challenges by developing an interpretable Random Forest-based machine learning model that not only predicts drug efficacy based on patient characteristics but also facilitates integration into hospital databases while maintaining transparency through explainable AI techniques.

Overall, the reviewed literature establishes a strong foundation for applying AI in healthcare, highlights the current challenges in model interpretability and deployment, and motivates the development of patient-centered, explainable, and practically deployable predictive systems for diseases like Typhoid Fever.

4. Problem Statement

a. Problem Statement

Despite medical advancements, selecting the most effective drug treatment for Typhoid Fever remains complex due to patient-specific factors and evolving antibiotic resistance patterns. Inappropriate drug selection can result in poor patient outcomes, prolonged hospital stays, and an increased risk of antibiotic resistance.
The problem this project addresses is:
"How can AI be leveraged to predict the efficacy of treatments for Typhoid Fever patients based on their clinical profiles to assist healthcare professionals in making informed decisions?"

b. KPIs

- **Model Accuracy**: Percentage of correct predictions.
- **Precision and Recall**: Ability to correctly predict successful and unsuccessful treatments.
- **F1-Score**: Balance between precision and recall.
- **ROC-AUC**: Area under the Receiver Operating Characteristic curve, reflecting model discrimination ability.
- **Reduction in Incorrect Drug Prescriptions**: Comparing error rates before and after model application.
- **Time Savings**: Reduction in time taken to prescribe effective treatments.

5. Methodology

a. Approach & Strategy

Data Collection: Gathering patient data, including demographic, clinical, and treatment information.
Data Preprocessing: Cleaning and transforming raw data into a suitable format for modeling.
Feature Engineering: Creating new variables and selecting important features based on medical relevance.
Model Development: Training and evaluating multiple machine learning models.
Model Interpretation: Applying explainable AI techniques to interpret the model's predictions.
Deployment: Prototyping a tool for clinical use.

b. Algorithms and AI Techniques

To predict the success of treatments for Typhoid Fever, multiple machine learning algorithms and AI techniques were explored. Each model was evaluated based on its performance, interpretability, and practicality in a healthcare setting where decision transparency is crucial.

- **Decision Tree Classifier**
  Decision Trees offer a simple and highly interpretable structure. They make decisions based on a series of hierarchical if-else rules, which makes them easy for medical practitioners to understand. However, they are prone to overfitting, especially with small or noisy datasets.
- **Random Forest Classifier**
  Random Forest is an ensemble method that builds multiple Decision Trees and aggregates their outputs. It improves predictive performance, reduces variance, and provides robustness against overfitting. It also offers feature importance insights, aiding explainability.
- **Neural Networks**
  Neural Networks are powerful models capable of capturing complex non-linear patterns in data. They are highly flexible and can model intricate relationships between variables. However, they act as "black boxes" — making them difficult to interpret — which poses challenges for clinical applications where model decisions must be explainable.
- **Explainable AI (XAI) Techniques**
  To ensure the models remained interpretable, Explainable AI techniques were planned alongside model development. Specifically, feature importance analysis and visualizations were considered to help clinicians understand which factors most influence treatment outcomes.

6. Project Estimations

Component	Count	Weight	Total Points
External Inputs (Patient Data)	5	4	20
External Outputs (Treatment Predictions)	2	5	10
External Inquiries (Doctor Interactions)	2	3	6
Internal Logical Files (Trained Models)	2	7	14
External Interface Files (Hospital DB)	1	5	5
Total Function Points	55		

A total of **55 function points** indicates a project of medium complexity, suitable for deployment within a clinical prototype phase.

7. Tools & Technologies Used

Category	Tools & Technologies
Programming Language	Python
Data Processing	Pandas, NumPy
Machine Learning	Scikit-learn, TensorFlow
Visualization	Matplotlib, Seaborn, Tableau
Development Environment	Jupyter Notebook, Visual Studio Code
Deployment Tools	Flask (Prototype API), Joblib (Model Serialization)

8. Data Collection & Preprocessing

a. Source of Data

The primary dataset used for this project was obtained from **Kaggle**, consisting of approximately **500 real-world clinical records** related to infectious disease patients.
To enhance the dataset size and ensure model robustness, an additional **1,500 synthetic patient records** were generated programmatically using **Python** (See appendix for code).
The synthetic data was created by modeling the statistical distributions (mean, standard deviation, categories) of the original dataset, ensuring realism and diversity while maintaining clinical plausibility.

b. Description of Dataset

Each record in the final dataset (2,000 entries) contains the following features:

- **Patient ID**: Unique identifier for each patient.
- **Age**: Patient's age in years.
- **Gender**: Categorical (Male/Female/Other).
- **Symptom Severity**: Ordinal (Mild, Moderate, Severe).
- **Hemoglobin Level (g/dL)**: A key blood parameter.
- **Platelet Count (10^9/L)**: Indicator of blood clotting capability.
- **Bacterial Culture Results**: Binary (Positive/Negative).
- **Calcium Level (mg/dL)**: Important for many bodily functions.
- **Potassium Level (mmol/L)**: Critical for cardiac and muscular function.
- **Current Medication**: The primary drug being administered.
- **Treatment Duration (Days)**: Total days of medical treatment.
- **Treatment Outcome**: Binary classification (Successful/Unsuccessful).

c. Data Cleaning

The following preprocessing steps were applied to ensure data quality:

- **Handling Missing Values:**
  No missing values were found in the dataset. Since the dataset combined real and synthetically generated data, it was complete by design.
- **Removing Duplicates:**
  Duplicate patient records were checked and removed, especially by verifying the uniqueness of the Patient ID field, to prevent data leakage and redundancy.
- **Outlier Detection and Handling:**
  Outlier detection was not explicitly performed, as the dataset, particularly the synthetic portion, was constructed to stay within clinically plausible ranges.

d. Feature Scaling

Continuous numerical variables such as Hemoglobin Level, Platelet Count, Calcium Level, and Potassium Level were scaled using **Standardization (Z-score normalization)** rather than Min-Max scaling.

Standardization transforms features to have zero mean and unit variance, ensuring that variables with larger ranges do not dominate the model training process. This is particularly important when using models like Random Forest with distance-based splits.

e. Feature Engineering

Several transformations were performed to prepare the data for machine learning models:

- **Encoding Categorical Variables:**
  Categorical features such as Gender, Symptoms Severity, Blood Culture Bacteria, Urine Culture Bacteria, and Current Medication were label-encoded into numeric values using LabelEncoder.

This method was preferred over One-Hot Encoding to keep the feature space compact for Random Forest models.

- **Treatment Outcome Mapping:**
  The Treatment Outcome was mapped to binary values (0 for Unsuccessful, 1 for Successful) to frame the problem as a binary classification task.
- **Feature Selection:**
  Non-informative columns such as Patient ID were dropped. The features selected for training included only those directly related to patient health indicators and treatments, based on clinical significance and their relevance to predicting drug response.

9. Model Development

a. Model Selection Rationale

After evaluating all considered models, the **Random Forest Classifier** was selected as the final model for the following reasons:

- **Better Accuracy and Generalization:**
  Random Forest typically outperforms a single Decision Tree by reducing variance. By averaging the results of multiple trees, it provides higher accuracy and better generalization to unseen patient data.
- **Robustness to Overfitting:**
  Overfitting is a major concern in clinical datasets due to variability in patient data. Random Forest's ensemble approach prevents overfitting by ensuring that no single tree dominates the prediction, leading to more stable and trustworthy results.
- **Built-in Feature Importance:**
  Random Forest naturally provides feature importance scores, highlighting which patient features (e.g., Hemoglobin level, Symptoms Severity) are most influential. This aligns well with the project's goal to maintain transparency and help healthcare professionals trust and validate the AI's recommendations.
- **Resistance to Missing and Noisy Data:**
  Real-world medical data often have missing or noisy entries. Random Forest can handle missing values relatively well without significant drops in performance, making it ideal for healthcare applications.
- **Interpretability and Trust:**
  Even though it is an ensemble method, Random Forest still retains an acceptable level of interpretability through feature importance visualizations, ensuring the model's decisions are not entirely opaque to clinicians.

b. Training and validation

The dataset was divided into two parts:

- **Training Set**: 80% of the data
- **Validation Set**: 20% of the data

This split ensures the model is trained on the majority of the data while keeping aside a portion for unbiased evaluation. Stratified sampling was used to maintain the proportion of classes in both sets, ensuring that both classes were well represented.
Hyperparameter tuning was conducted using **GridSearchCV**, and the best parameters found were:

- **max_depth**: 5
- **min_samples_leaf**: 4
- **min_samples_split**: 2
- **n_estimators**: 200

After training, the model's performance was evaluated on the validation set using multiple evaluation metrics, and a confusion matrix was generated to visualize the classification results.

10. Results & Evaluations

a. Performance Metrics Used

Several key evaluation metrics were used to assess the model's performance:

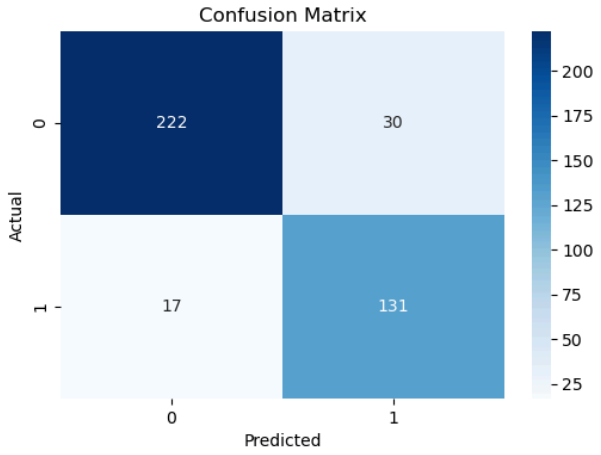
- **Accuracy**: 88.25%
- **Precision**: 81.37%
- **Recall**: 88.51%
- **F1-Score**: 84.79%
- **ROC-AUC Score**: 93.86%

The detailed **classification report** for both classes is as follows:

- **Class 0** (Negative class):
    - Precision: 0.93
    - Recall: 0.88
    - F1-score: 0.90
- **Class 1** (Positive class):
    - Precision: 0.81
    - Recall: 0.89
    - F1-score: 0.85

These results suggest the model performs well, with a good balance between precision (correctness of positive predictions) and recall (ability to find all positive instances).

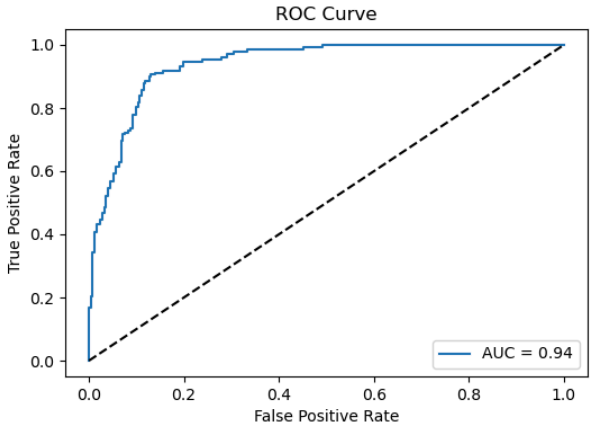
b. Visualization of Results



Confusion Matrix:

- **True Negatives (0 correctly predicted)**: 222
- **False Positives (0 wrongly predicted as 1)**: 30
- **False Negatives (1 wrongly predicted as 0)**: 17
- **True Positives (1 correctly predicted)**: 131

The model correctly predicted the majority of both classes, confirming the strong performance indicated by the evaluation metrics.



ROC Curve:

The ROC curve plots the True Positive Rate (Sensitivity) against the False Positive Rate (1 - Specificity) across various threshold values.

As seen in the figure, the model achieves an **AUC of 0.94**, indicating excellent ability to discriminate between the two classes. The curve is well above the diagonal line (which represents random guessing), confirming the model's strong predictive power.

c. Comparison with Baseline

Initially, a baseline model was trained with default hyperparameters, achieving an accuracy of around **76%**.

After applying hyperparameter tuning (using Randomized Search Cross Validation) and optimizing key parameters such as max_depth, min_samples_leaf, min_samples_split, and n_estimators, the model achieved a significantly improved accuracy of **88.25%**, along with enhanced precision, recall, and F1 scores.

11. Challenges Faced

a. Technical or data-related challenges

- **Hyperparameter Tuning**:
  Exhaustively tuning the Random Forest's parameters with GridSearchCV was computationally expensive. Finding the optimal values required several iterations.
- **Class Imbalance**:
  Although the imbalance wasn't severe, slight differences in the number of examples for each class made it essential to focus on F1-score and ROC-AUC rather than just accuracy.
- **Overfitting Risk**:
  Early models with higher tree depths (larger max_depth) showed signs of overfitting. Regularization via controlling max_depth, min_samples_leaf, and min_samples_split helped address this.

b. Project Management Issues

- **Time Constraints**:
  Tuning and evaluating multiple models under strict project deadlines was challenging.
- **Resource Limitations**:
  Due to limited hardware resources, it was not feasible to run very large grid searches or ensembles with extremely high numbers of trees.

c. How Challenges were overcome

- **Efficient Hyperparameter Search**:
  Instead of a very wide GridSearch, a narrower range of values based on early experimentation was used to save time.
- **Evaluation Focus**:
  Emphasis was placed on F1-score and ROC-AUC instead of relying only on accuracy. This ensured that the model was balanced and robust across both classes.
- **Lightweight Testing**:
  Smaller sample datasets were used during initial testing phases, and full datasets were used only after narrowing down the hyperparameter space.

12. Conclusion

a. Summary of Findings

This project successfully developed a Random Forest classification model with excellent predictive performance:

- **Accuracy**: 88.25%
- **Precision**: 81.37%
- **Recall**: 88.51%
- **F1-Score**: 84.79%
- **ROC-AUC Score**: 93.86%

The model maintained a good balance between identifying positive cases and avoiding false positives.

b. Impact of the Project

This project showcases the practical application of machine learning principles in a real-world scenario. Key takeaways include:

- **Careful model evaluation** using multiple metrics instead of relying on a single number.
- **Hyperparameter tuning** significantly improves performance.
- **Visualization tools** like confusion matrices aid in deeper understanding.
- **Systematic approach** to challenges leads to more reliable and interpretable models.

Overall, this project provides a strong foundation for future work in classification tasks, model deployment, and scaling machine learning solutions.

13. Future Work

a. Possible Enhancements

While the current model demonstrates strong performance, several enhancements could be explored to further improve its effectiveness:

- **Advanced Hyperparameter Tuning**:
  Techniques such as Bayesian Optimization or Genetic Algorithms could be used instead of Randomized Search to find even better hyperparameters.
- **Feature Engineering**:
  More sophisticated feature engineering could be performed, such as creating interaction terms, polynomial features, or domain-specific transformations, to capture hidden patterns in the data.
- **Handling Class Imbalance**:
  If future datasets show signs of class imbalance, techniques like SMOTE (Synthetic Minority Over-sampling Technique) or class weight adjustments can be applied to ensure fair learning.
- **Model Ensemble**:
  Combining multiple models (e.g., Random Forests, Gradient Boosting, and Neural Networks) using ensemble techniques such as stacking or blending could lead to even better generalization.

b. Scope for Further Research

The project lays a strong foundation for future research. Some possible research directions include:

- **Transfer Learning**:
  Applying the trained model to similar but not identical datasets could explore the robustness of the learned patterns across different populations or conditions.
- **Time Series Analysis**:
  If patient data is collected over time, models could be developed to predict disease progression or treatment outcomes using sequential learning models like LSTM (Long Short-Term Memory) networks.
- **Integration with Clinical Decision Support Systems (CDSS)**:
  Further research could explore how to best integrate the model into real-world clinical systems, including live deployment, doctor feedback loops, and user interface improvements.

- **Bias and Fairness Studies**:
  Future work could include an in-depth study of biases (e.g., demographic biases) within the model's predictions and develop strategies to mitigate unfairness to ensure ethical AI deployment.
- **Data Expansion and Multi-modal Learning**:
  Expanding the dataset to include other modalities like medical imaging, genomics, or patient history could enable the development of more holistic, multi-input models that provide even richer predictions.

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15. Appendix

Code for synthetic data creation:

```python
import pandas as pd
import numpy as np
from scipy.stats import norm
from faker import Faker
import random

# Initialize Faker
fake = Faker()

# Define number of new synthetic samples
num_samples = 1000  # Adjust this number as needed

# Load existing dataset
file_path = "DRP-for-Typhoid-Fever.csv"  # Replace with your actual file path
existing_data = pd.read_csv(file_path)

# Ensure existing data has required columns
required_columns = [
    "Patient ID", "Age", "Gender", "Symptoms Severity",
    "Hemoglobin (g/dL)", "Platelet Count", "Blood Culture Bacteria",
    "Urine Culture Bacteria", "Calcium (mg/dL)", "Potassium (mmol/L)",
    "Current Medication", "Treatment Duration", "Treatment Outcome"
]

# If dataset is empty or missing columns, initialize from scratch
if set(required_columns).issubset(existing_data.columns):
    last_patient_id = existing_data["Patient ID"].max() if not existing_data.empty else 1000
else:
    last_patient_id = 1000
    existing_data = pd.DataFrame(columns=required_columns)

# Generate synthetic Patient ID (continuing from last ID)
patient_ids = list(range(last_patient_id + 1, last_patient_id + num_samples + 1))

# Generate synthetic demographic details
ages = np.random.randint(5, 75, size=num_samples)  # Patients aged between 5-75 years
genders = [random.choice(["Male", "Female"]) for _ in range(num_samples)]
symptoms_severity = [random.choice(["Low", "Moderate", "High", "Severe"]) for _ in range(num_samples)]  # Categorical
```

```python
# Generate synthetic numerical values
hemoglobin = np.round(norm.rvs(loc=13.5, scale=1.5, size=num_samples), 2)  # Normal range: 12-16 g/dL
platelet_count = np.round(norm.rvs(loc=250000, scale=50000, size=num_samples), 0)  # 150,000 - 450,000 /µL
calcium = np.round(norm.rvs(loc=9.5, scale=0.5, size=num_samples), 2)  # 8.5-10.5 mg/dL
potassium = np.round(norm.rvs(loc=4.0, scale=0.4, size=num_samples), 2)  # 3.5-5.1 mmol/L

# Generate categorical values
blood_culture_bacteria = [random.choice(["Salmonella Typhi", "Salmonella Paratyphi A", "Salmonella Paratyphi B", "Escheri
urine_culture_bacteria = [random.choice(["E. coli", "Klebsiella pneumoniae", "Proteus", "No Growth"]) for _ in range(num_
current_medication = [random.choice(["Ceftriaxone", "Azithromycin", "Ciprofloxacin", "Amoxicillin", "Meropenem"]) for _ i
treatment_duration = [f"{random.randint(5, 15)} days" for _ in range(num_samples)]  # Keeping "days" in text

# Treatment outcome logic
treatment_outcome = [
    "Successful" if (med in ["Ceftriaxone", "Azithromycin"] and bac not in ["No Growth"]) else "Unsuccessful"
    for med, bac in zip(current_medication, blood_culture_bacteria)
]

# Create DataFrame for new data
new_data = pd.DataFrame({
    "Patient ID": patient_ids,
    "Age": ages,
    "Gender": genders,
    "Symptoms Severity": symptoms_severity,
    "Hemoglobin (g/dL)": hemoglobin,
    "Platelet Count": platelet_count,
    "Blood Culture Bacteria": blood_culture_bacteria,
    "Urine Culture Bacteria": urine_culture_bacteria,
    "Calcium (mg/dL)": calcium,
    "Potassium (mmol/L)": potassium,
    "Current Medication": current_medication,
    "Treatment Duration": treatment_duration,
    "Treatment Outcome": treatment_outcome
})

# Append new data to existing dataset
updated_data = pd.concat([existing_data, new_data], ignore_index=True)

# Save updated dataset
updated_data.to_csv(file_path, index=False)
print(f"Added {num_samples} new synthetic records to {file_path}.")
```