

Predictive modeling of antimicrobial resistance in zoonotic *Salmonella enterica*: a retrospective machine learning analysis of national surveillance data (2000–2020)

Modelización predictiva de la resistencia antimicrobiana en *Salmonella entérica* zoonótica: un análisis retrospectivo mediante aprendizaje automático de datos nacionales de vigilancia (2000–2020)

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ABSTRACT

Zoonotic pathogens are an important One Health issue from the perspective of antimicrobial resistance. However, surveillance datasets remain underutilized in this area, which can lessen the risks linked to antimicrobial resistance. This research examined how well machine learning techniques could accurately predict tetracycline resistance in *Salmonella enterica* isolates obtained from veterinary sources. Data collected between 2000 and 2020 from the Food and Drug Administration national antimicrobial resistance monitoring system was studied. This article focused on developing a classification-based predictive model for the classification of serovars of salmonella pathogens using machine-learning tools. Through using 5-fold stratified cross-validation was conducted for model performance evaluation along with clinical utility via prevailing negative predictive value and 95% confidence intervals. Tetracycline resistance was found to be overall 12.7%. The predictive performance of XGBoost was the best at AUC = 0.817 (95% CI: 0.802–0.829) than logistic regression (0.790). The internal stability of the model was strong and the negative predictive value was 94.9%, a good identification of susceptible isolates. Analysis of feature importance of resistance indicated that serotype was the most important variable, followed by temporal and spatial variables. The results shed light on the potential of gradient-boosted models for antimicrobial resistance risk stratification for antimicrobial resistance issues as well as antimicrobial stewardship, especially in the setting of guiding empirical therapy in the absence of laboratory results.

Key words: Antimicrobial resistance; Machine learning; *Salmonella*; One Health; XGBoost; Veterinary informatics

RESUMEN

Los patógenos zoonóticos representan un desafío clave para el enfoque One Health (Una Sola Salud), especialmente con respecto a la resistencia a los antimicrobianos. No obstante, los datos de vigilancia disponibles continúan estando infrautilizados, lo que dificulta la mitigación efectiva de los riesgos asociados a la resistencia a los antimicrobianos. La investigación se realizó con el objetivo de evaluar el potencial de técnicas de aprendizaje automático para predecir con precisión la resistencia a la tetraciclina en aislamientos de *Salmonella entérica* procedentes de fuentes veterinarias. Para ello, se analizaron datos recopilados entre 2000 y 2020 por el Sistema Nacional de Monitoreo de la Resistencia a los Antimicrobianos de la Administración de Alimentos y Medicamentos de los Estados Unidos. El estudio se centró en desarrollar un modelo predictivo de clasificación para la identificación de serovares de *Salmonella* mediante técnicas de aprendizaje automático. Para evaluar el rendimiento, se utilizó una validación cruzada estratificada de 5 pliegues. Además, se analizó la utilidad clínica a través del valor predictivo negativo, con intervalos de confianza del 95 %. La resistencia a la tetraciclina se estimó en un 12,7 % en general. El modelo XGBoost presentó el mejor rendimiento predictivo con un AUC = 0,817 (IC 95 %: 0,802–0,829), en comparación con la regresión logística (0,790). La estabilidad interna del modelo fue sólida y el valor predictivo negativo alcanzó el 94,9 %, indicando una buena identificación de los aislamientos susceptibles. El análisis de la importancia de las variables reveló que el serotipo fue el factor más relevante, seguido de variables temporales y espaciales. El estudio mostró el potencial de los modelos de *gradient boosting* para la estratificación del riesgo de resistencia a los antimicrobianos, así como para la gestión responsable de antimicrobianos, sobre todo en la orientación de terapias empíricas en ausencia de resultados de laboratorio.

Palabras clave: Resistencia antimicrobiana; Aprendizaje automático; *Salmonella*; One Health; XGBoost; Informática veterinaria

INTRODUCTION

Antimicrobial resistance (AMR) is an invisible pandemic that threatens both animal health and food security and public health [1]. The Veterinary sector is an important part of the AMR ecosystem. The use of antimicrobials in food-producing animals may select for resistant bacteria with zoonotic ability. These can be transferred to humans [2].

Salmonella enterica is a kind of bacterium that is one of the most important zoonotic pathogens for humans and other animals [3]. The emergence of multidrug-resistant strains, such as tetracycline and fluoroquinolone-resistant *Salmonella*, complicates empirical treatment and requires the proper surveillance [4].

National surveillance programs have generated large databases of phenotypic resistance data including the National Antimicrobial Resistance Monitoring System (NARMS) in the US and European Surveillance of Veterinary Antimicrobial Consumption [5]. Still, the use of this data has mostly been retrospective and descriptive. Traditionally, epidemiological reports summarize resistance prevalence by year or commodity which makes it difficult to identify trends as they arrive [6].

Although useful for developing policies, these descriptive methods do not have the forecasting capacity for proactive clinical action. Clinicians and policymakers will find a useful tool to help predict possible resistance phenotypes based on easily accessible risk factors, such as the animal host, geographical region, bacterial serotype [7].

The use of Artificial intelligence and machine learning (ML) can be helpful in bridging the gap between raw surveillance data and actionable intelligence [8]. ML algorithms can detect disease linkages from epidemiological variables due to their capacity to model complex non-linearities in high-dimensional data to optimize predictive accuracy, unlike classical statistical techniques, such as logistic regression, which rely on linear assumptions and do poorly at high-dimensional interaction [9, 10].

According to recent studies in Human Medicine, ML has the ability to predict AMR phenotypes from genomic data [11]. However, such techniques have yet to be applied to any phenotypic Veterinary surveillance data. Accordingly, the aim of this study was to develop and validate a machine learning framework for the prediction of antimicrobial resistance in Veterinary *Salmonella* isolates.

So, the objectives of the present study, were to (1) investigate the performance of classical models and ML algorithms (Random Forest and XGBoost), (2) identify the epidemiological drivers of tetracycline resistance, and (3) evaluate the clinical usefulness of these models as screening tools for antimicrobial stewardship.

MATERIALS AND METHODS

Data source and study population

Data on retrospective antimicrobial susceptibility were retrieved through the FDA NARMS Integrated Dataset, which is a compilation of routine surveillance isolates (Veterinary, food and public health) in the United States [12]. The data set comprised *S. enterica*

isolates that were obtained in 2000–2020. The target population included isolates of the animals of significant food production of cattle (*Bos taurus*), swine (*Sus scrofa domesticus*), poultry (*Gallus gallus domesticus*) and companions.

To find the prevalence percentage, the number of resistant isolates was divided by the total number of isolates and multiply by 100.

Inclusion and exclusion criteria

The analysis included isolates that had full metadata of serotype, year of collection, and geographical area. To make the analysis narrow down to the clinically relevant pathogens, the dataset with the 20 most common *Salmonella* serotypes occurring in the Veterinary industry was filtered. Phenotypic resistance to Tetracycline, which is a central indicator antibiotic to be used by the Veterinarians, was used as the primary outcome variable [13]. The resistance was determined as a dichotomous classification (Resistant vs. Susceptible) according to Clinical and Laboratory Standards Institute breakpoints in the data set [14]. The result of the isolates of the intermediate susceptibility was excluded to guarantee a binary classification rigor.

Machine learning algorithms

Four distinct classification algorithms were implemented to evaluate predictive performance:

- **Logistic Regression (LR):** Employed as the standard epidemiological baseline to establish linear associations [15].
- **Decision Tree (DT):** Utilized for its high interpretability and ability to generate visual decision rules [16]. The simplified clinical decision tree for resistance prediction is shown in FIG. 1.
- **Random Forest (RF):** An ensemble learning method based on bagging to reduce variance and prevent overfitting [17].
- **Extreme Gradient Boosting (XGBoost):** An advanced ensemble method utilizing gradient boosting to correct prediction errors iteratively [18].

Model validation and statistical analysis

The dataset ($n = 26,230$) was partitioned into a training set (70%) and a held-out test set (30%) using stratified random sampling to maintain the prevalence of resistance across splits. Internal validation was performed using stratified 5-fold cross-validation on the training set.

Model performance was assessed using Area Under the Receiver Operating Characteristic Curve (AUC-ROC), Sensitivity, Specificity, Positive Predictive Value, and Negative Predictive Value (NPV). Statistical robustness of the AUC scores was determined using bootstrap analysis ($n = 1,000$ iterations). All analyses were conducted using Python (v3.10) with the Scikit-learn and XGBoost libraries.

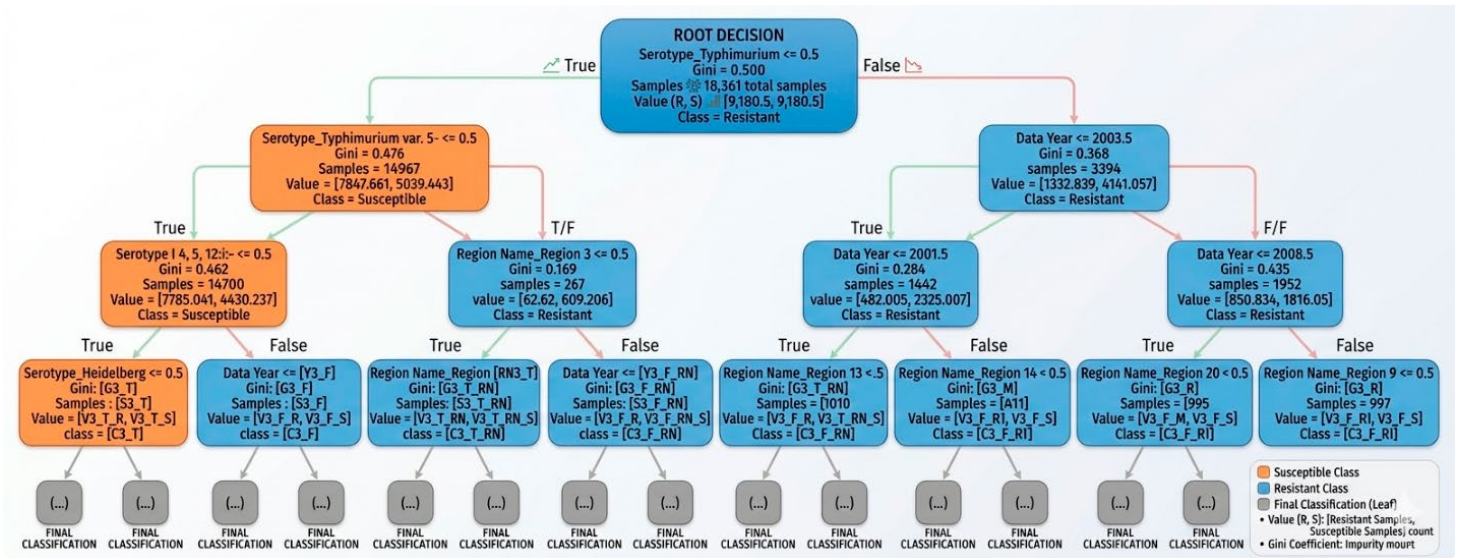


FIGURE 1: Simplified clinical decision tree for resistance prediction. A pruned decision tree visualizing the hierarchical interaction of risk factors

RESULTS AND DISCUSSION

Descriptive epidemiology

In the present study, 26,230 *Salmonella* isolates were included in the final analysis. The overall of tetracycline resistance obtained in this study population was 12.7% (TABLE I). As it can be observed in FIG. 2, bacterial serotype significantly influenced the distribution of resistance. The strains responsible for the greatest level of resistance recorded in the dataset was *S. Typhimurium* and its variants.

The serotype's association with *Typhimurium* and related variants agrees with earlier epidemiological data, which indicate that these strains are frequently associated with antimicrobial

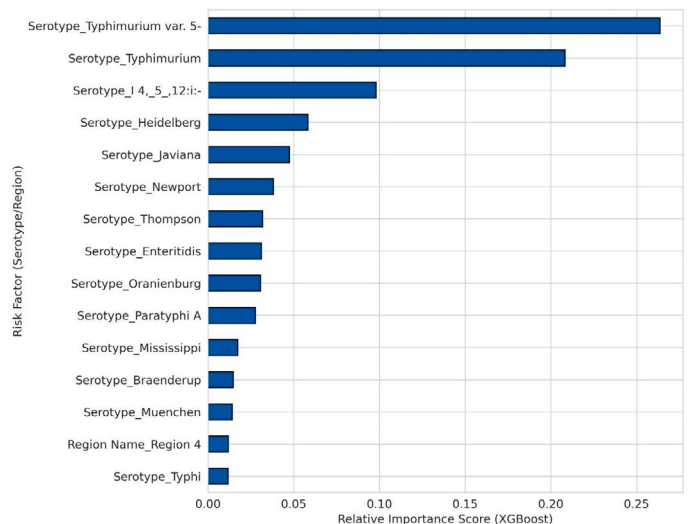


FIGURE 2: Top 15 Predictors of Resistance (Feature Importance). Bacterial serotype classification was identified as the dominant driver of resistance phenotypes

resistance determinants and commonly related to production systems involving livestock [19, 20].

Variability in resistance across serotypes likely reflects differences in the distribution of resistance genes and mobile genetic elements among *Salmonella* lineages, as well as differences in selective pressures in animal production environments. These findings highlight the importance of considering bacterial population structure when modeling antimicrobial resistance patterns.

Comparative model performance

The performance of the four algorithms evaluated in this study is summarized in TABLE II. Among the tested approaches, the XGBoost model demonstrated the highest discriminative ability

Characteristic	Total Isolates (n)	Resistant Isolates (n)	Prevalence (%)
Overall Population	26,230	3,331	12.7%
Top 5 Serotypes			
<i>S. Typhimurium</i>	4.21	1,052	25.0%
<i>S. Newport</i>	2.845	455	16.0%
<i>S. Heidelberg</i>	1.98	316	16.0%
<i>S. Infantis</i>	1.56	187	12.0%
<i>S. Enteritidis</i>	1.42	85	6.0%
Collection Period			
2000 – 2005	6.54	981	15.0%
2006 – 2010	6.21	745	12.0%
2011 – 2015	6.85	753	11.0%
2016 – 2020	6.63	852	12.9%

TABLE II
Comparative performance metrics of four machine learning algorithms in predicting tetracycline resistance on the held-out test set (n = 7,869)

Model	AUC (95% CI)*	Accuracy (%)	Sensitivity (Recall) (%)	Specificity (%)	NPV* (%)
XGBoost	0.817 (0.802–0.829)	79.0%	68.6%	80.5%	94.9%
Logistic Regression	0.790 (0.775–0.805)	76.0%	65.2%	77.8%	93.8%
Random Forest	0.783 (0.768–0.798)	78.0%	62.1%	79.5%	93.1%
Decision Tree	0.761 (0.745–0.777)	79.5%	58.4%	82.1%	92.5%

AUC: Area Under the Curve; CI: Confidence Interval; NPV: Negative Predictive Value

(FIG. 3), achieving an AUC of 0.817 (95% CI: 0.802–0.829). The superior performance of the XGBoost model observed in this study is consistent with previous reports demonstrating its effectiveness for antimicrobial resistance prediction. Unlike traditional statistical approaches, XGBoost can model complex nonlinear interactions among epidemiological, temporal, and environmental variables while minimizing overfitting through regularization techniques [21]. However, the differences between models were relatively small. Logistic regression and random forest models showed slightly lower performance (AUC = 0.790 and 0.783, respectively), while the decision tree model exhibited the lowest predictive accuracy (AUC = 0.761).

The superior performance of XGBoost suggests that gradient-boosted decision tree algorithms are particularly well suited for predicting antimicrobial resistance using surveillance data. Antimicrobial resistance epidemiology is inherently complex and often involves non-linear interactions among bacterial genetics, host species, and environmental factors.

Boosting algorithms such as XGBoost are capable of capturing these interactions through iterative model optimization, which

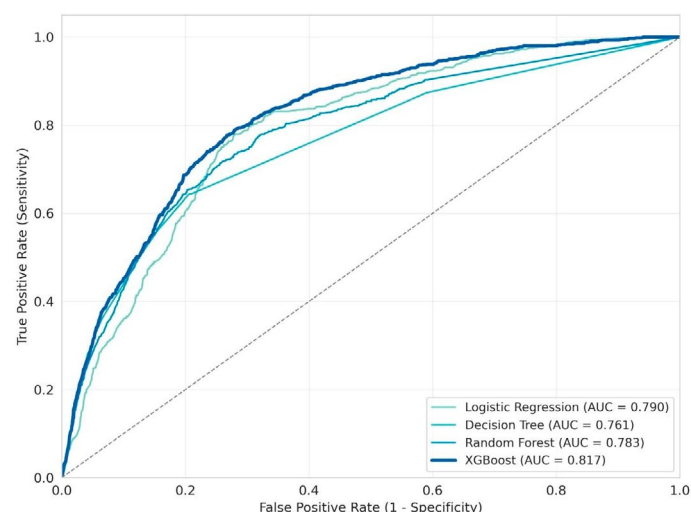


FIGURE 3: Comparative Receiver Operating Characteristic (ROC) curves for four classification algorithms. The XGBoost model (dark blue line) demonstrated superior discriminative ability

may explain their improved predictive performance compared with traditional regression-based approaches [21, 22].

Clinical utility and model calibration

When the held-out test dataset was used, the XGBoost model had a negative predictive value (NPV) of 94.9%. It means nearly 95% of isolates that were predicted to be susceptible were indeed susceptible (TABLE II)

Calibration curve given in FIG. 4, showed the level of agreement between predicted probabilities and observed outcomes. The high NPV is especially important for decision-making from a clinical perspective. In veterinary practice, empirical antimicrobial therapy is often initiated in order to achieve timely treatment and maintain animal welfare [23]. For this reason, the model's ability to reliably identify isolates likely to be susceptible could more accurately inform empirical treatment decisions. The model's low positive predictive value can be attributable to the lower prevalence of tetracycline resistance in the dataset. This behaviour is likely still advantageous. This is because when isolates are predicted to have increased probability of resistance, they can be prioritized for confirmatory susceptibility testing. Thus, this is beneficial for AM stewardship and unnecessary antimicrobial exposure [24, 25].

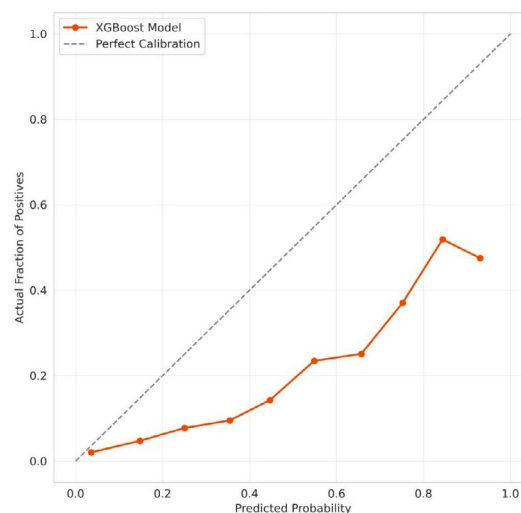


FIGURE 4: Reliability Curve (Calibration plot) of the XG Boost model. The model in orange line tracks the ideal diagonal, indicating reliable risk probability estimates

Risk factor analysis

The fluctuating prevalence of tetracycline resistance over the study period is shown in FIG. 5. From 2000 to 2011, tetracycline resistance among the sampled isolates declined substantially. However, from 2012 onwards, a slight rebound was observed. Analysis of feature importance provided by XGBoost model suggested that the most important predictor of tetracycline resistance is bacterial serotype (TABLE III). Specifically, *S. Typhimurium* var 5-, *S. Typhimurium*, and *S. Heidelberg*, had a strong association with phenotypic resistance. This result is in line with the findings of Carroll *et al.* [26].

TABLE III
Top 5 Predictors of Tetracycline Resistance identified by the XGBoost Model (Feature Importance Ranking)

Rank	Feature Name	Relative Importance Score	Clinical Interpretation
1	Serotype: <i>S. Typhimurium</i> var. 5-	0.264	Highest association with resistance
2	Serotype: <i>S. Typhimurium</i>	0.208	Strong association with resistance
3	Serotype: <i>S. I 4,[5], 12:i:-</i>	0.088	Moderate association
4	Serotype: <i>S. Heidelberg</i>	0.058	Moderate association
5	Serotype: <i>S. Newport</i>	0.049	Moderate association

This study showed the newly discovered gene, *mcr-9*, in *Salmonella Typhimurium*, confers phenotypic resistance to colistin in Enterobacteriaceae. Thus, this is a public health threat. The study's results reinforce the pivotal role played by bacterial lineage in determining antimicrobial resistance patterns. The accumulation of resistance genes within *Salmonella* populations and their niches could be responsible for serotype-specific resistance profiles. By integrating these epidemiological indicators into a prediction model, we may better identify isolates at high risk of resistance.

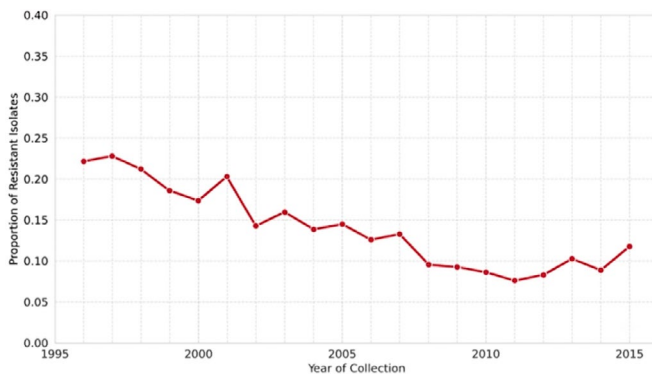


FIGURE 5: Temporal Trend of Tetracycline Resistance (2000–2020)

CONCLUSION

The study revealed that the use of retrospective surveillance data as stewardship tools is possible through machine learning. Among the evaluated algorithms, XGBoost model provided a highly accurate and safe method to predict tetracycline resistance in zoonotic *Salmonella*. The high negative predictive value (94.9%) demonstrated the model's ability to accurately identify susceptible isolates. As a result, these findings enhance the application of AI-driven clinical decision support systems in veterinary practice to improve treatment outcomes and public health protection.

Limitations

There are a number of limitations in this study. To begin with, the analysis relied on surveillance data sourced passively. This could

potentially have a sampling bias and furthermore, does not contain detailed information on antimicrobial use or clinical outcomes. Another factor is that while the NARMS dataset is geographically representative in the United States, we are unsure how well this model applies to other areas or production systems. Future work can utilize other epidemiological data like farm-level antimicrobial-usage data to refine its predictive power and external validation.

Ethics approval

As this study did not involve human or animal subjects, approval from an Institutional Animal Care and Use Committee or Institutional Review Board was not required.

Availability of data and materials

The data used in the current study is publicly available. They were obtained from the NARMS, a publically available surveillance program jointly administered by the U.S. Food and Drug Administration (FDA), the Centers for Disease Control and Prevention (CDC) and the U.S. Department of Agriculture (USDA). The primary dataset is accessible on: <https://goo.su/hOepq0>

Conflict of interest statement

The authors declare that they have no conflict of interest.

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