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Integrating Clinical Markers and Machine Learning for Accurate Prediction of Neonatal Sepsis

Dr. Lilly Sheeba S[1], Ms. Faritha Begum M[2], Ms. Preethi Parameswari S[3], Ms. Rachel Evelyn R[4], Ms. Sangeetha N[5], Ms. Sandhiyaa S[6]

[1]Professor, Department: Cyber Security, Jerusalem College of Engineering, Chennai, Tamil Nadu, India
ORC id: 0000-0002-9465-1300
Email ID: lillysheeba1@gmail.com
[2]Assistant Professor, Department: Cyber Security, Jerusalem College of Engineering, Chennai, Tamil Nadu, India
Email ID: farithait14@gmail.com
[3]Assistant Professor, Department: Cyber Security, Jerusalem College of Engineering, Chennai, Tamil Nadu, India
ORC id: 0000-0002-7142-3700
Email ID: preethiparameswari8@gmail.com
[4]Assistant Professor, Department: Cybersecurity, Jerusalem College of Engineering, Chennai, Tamil Nadu, India
Email ID: rachelevelyn12@gmail.com
[5]Assistant Professor, Department: Cyber Security, Jerusalem College of Engineering, Chennai, Tamil Nadu, India
Email ID: sanrai2799@gmail.com
[6]Assistant Professor, Department: Cyber Security, Jerusalem College of Engineering, Chennai, Tamil Nadu, India
Email ID: sandhiyaascs@jerusalemengg.ac.in

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ABSTRACT

Background: clinically suspected sepsis is a common occurrence in preterm and severely unwell newborns during their extended stay in the neonatal intensive care unit (NICU). This might be the first indicator of further negative outcomes. Consequently, our objective was to use data-driven learning techniques to forecast newborn in-hospital mortality using machine learning methods. The methodology included enrolling 1095 newborns who were admitted to a tertiary-level neonatal intensive care unit (NICU) in Taiwan from 2017 to 2020 for clinical suspicion of sepsis. Clinical symptoms, laboratory criteria, and the use of empiric antibiotics by doctors were used to define sepsis when it was clinically suspected. Patient demographics, clinical characteristics, laboratory data, and medicines were the variables used for analysis. Incorporating machine learning techniques, we employed DNN, k-nearest neighbours, support vector machine, random forest, and extreme gradient boost. We used the area under the receiver operating characteristic curve (AUC) to determine how well these models performed. Findings: 8.2% (90 newborns) died as a result of complications while in the hospital. The training set consisted of 765 patients (or 69.8% of the total) while the test set included 330 patients (or 30.2% of the total). Among the models that were evaluated for their ability to predict the outcome, DNN stood out with the highest area under the curve (0.923, 95% CI 0.953-0.893), the best accuracy (95.64%, 95% CI 96.76-94.52%), and the best values for Cohen's kappa (0.74, 95% CI 0.79-0.69) and Matthews correlation (0.75, 95% CI 0.80-0.70). Ventilator support needs upon suspicion of sepsis, feeding circumstances, and intravascular volume expansion were the three most important factors in the DNN significance matrix plot. Neither the training nor the test sets showed any significant difference in the model's performance. Clinicians may benefit from the machine learning algorithm's insights and improved advance communication with families after establishing the DNN model to forecast in-hospital mortality in newborns with clinically indicated sepsis.

Keywords: *Neonatal mortality, AI, big data, neonatal sepsis, early prediction, and machine learning.*

1. INTRODUCTION

Even when patients overcome the most severely sick times during the perinatal periods, considerable mortality may occur in preterm newborns or high-risk neonates hospitalised in the neonatal intensive care unit (NICU) [1,2]. Various invasive infections are the most common cause of instability in these delicate individuals, while immature organ functions may play a role [3,4]. Due to their weak immune defences, protracted intubation and hospital stays, presence of artificial devices, and

underlying chronic illnesses, these patients are most susceptible to late-onset sepsis or clinical sepsis [4-6]. Reports indicate that hospitalised neonates in the NICU had an overall unadjusted in-hospital death rate ranging from 6.4% to 10.9% [1-3,7]. It is common for doctors to face clinically suspected sepsis in the NICU. This condition is characterised by clinically septic characteristics, aberrant laboratory results, and their judgements on whether to administer empiric antibiotics [8,9]. Clinicians and parents of very premature newborns may underestimate the unstable prematurity circumstances due to optimism bias and unanticipated mistake, which may delay crucial communication about the patient's prognosis during the over three-month duration of their hospital stay [10,11]. Current prognostic tools may be helpful, but they aren't applicable to all neonates in the NICU, and it might be a pain to enter all the data needed for them [12–15]. Machine learning (ML) techniques have recently been used to model nonlinear and linear characteristics for hospitalised patients, taking use of improved processing capability [16,17]. Predicting the beginning of sepsis, mortality, and morbidity using ML algorithms that use regularly gathered data and electronic records might help doctors make more suitable treatment choices [16-19]. Nevertheless, these ML algorithms have not yet been implemented for use with newborns coping with persistent comorbidities while in the hospital. Deep neural networks (DNNs) outperform other ML models when it comes to processing large amounts of medical data from sources like national or international databases, and they also have excellent interpretability and practicality [17]. To reliably predict the in-hospital mortality of newborns with clinically suspected sepsis in the NICU, we intended to construct a DNN-based multivariate regression model and evaluate it with six existing ML methods.

2. METHODOLOGY

2.1 Research Participants, Environment, and Methods

From August 2017 through July 2020, we examined a cohort of all newborns admitted to the neonatal intensive care units (NICUs) of Chang Gung Memorial Hospital (CGMH) with a recorded case of clinically suspected sepsis. There are a total of 58 beds available in special care nurseries and 49 beds with ventilators in the three NICU units at CGMH. Around 800 neonates are admitted to these NICUs at CGMH each year. Almost 30% of Taiwan's critically sick and preterm children are admitted to the neonatal intensive care units (NICUs) at CGMH, making them the biggest tertiary-level referral medical centre in the country.

Clinical and laboratory diagnoses were used to determine the presence of sepsis [8,9]. The following were part of the diagnostic criteria for "clinically suspected sepsis": 1. exhibiting a septic symptom, such as an unstable vital sign, apnoea, increased oxygenation support, tachycardia or bradycardia, reduced activity, vomiting, or poor intake; and 2. testing positive for a minimum of two of the following experimental tests: the number of white blood cells is abnormal (<5 × 10^6/L or > 20 × 10^6/L), the ratio of immature to total neutrophils is more than or equal to 0.1, the number of platelets is less than or equal to 100 × 10^6/L, the level of haemoglobin is less than or equal to 11.0 g/dL, and the level of C-reactive protein is greater than or equal to 6 mg/L. These unstable occurrences necessitated the collection of a blood sample and/or a sterile-site sample for culture, the administration of empirical antibiotics, and the invocation of ventilator support, cardiac inotropic medications, or volume expansion, among other forms of augmented life support. From the time of clinical suspicion of sepsis until discharge or death, we prospectively monitored all newborns. We didn't include newborns who passed away in the first week or had serious congenital defects. We only looked at each patient's first episode of instability. The infants were split up into two groups at random: with which to train ML models and with which to measure their performance. The Chang Gung Memorial Board's Institutional Review Board waived informed consent requirements for this research (certificate number. 201802021B0).

2.2 Research Factors and Data Preparation

We obtained baseline demographic information from each patient, which includes their birth weight, gestational age, gender, delivery method, pregnancy and postnatal history, and any comorbidities they may have.Neural consequences, bronchopulmonary dysplasia, congenital cardiac illness, cholestasis, renal function impairment, and gastrointestinal disorders were among the chronic comorbidities.

Prior to the start of these unpredictable occurrences, laboratory data was collected, including white blood cell count, haemoglobin, platelet count, blood gas analysis, C-reactive protein, electrolytes, bilirubin, and outcomes of renal and hepatic function. When all possible sterile locations were cultured and a laboratory assessment was conducted, it was considered the initial septic evaluation, marking the beginning of clinically suspected sepsis. Vital signs, heart rate (tachycardia or bradycardia), breathing patterns, dietary changes, medication use, chronic diseases, and the use of any prosthetic limbs were all documented as clinical symptoms. Mortality in the neonatal intensive care unit was the main endpoint, and the censoring of critical care cessation owing to family requests for transfers to other institutions was not.Numerical data and codes were assigned based on patient outcomes and a few non-numerical characteristics. The feature selection procedure made use of a newly created numerical dataset with 56 columns after the conversion. These columns included 55 variables in addition to the outcomes of all patients.

2.3 The Scoring Process

After plugging in the inputs, the scoring function estimated the output scores, which were then utilised to forecast the final results. A DNN model, which is both a reasonably established technology and has great nonlinear computing capabilities, was chosen as the scoring function in this study: [17]. Seventy percent of the infants recruited served as training subjects, while thirty percent served as test subjects. In this work, the DNN model is shown in Figure 1A. It consists of an input layer, three hidden layers, and an output layer. Each of the three buried levels included a different number of neurones: 128, 64, and 32. Further, in order to sidestep the vanishing gradient issue, the rectified linear unit (ReLU) was chosen as the activation function.

2.4 Scoring Procedure Choice of Features

We used the newborns' computed Pearson product-moment correlations (PPMCCs) as our defining characteristics. The feature selection method then moved on to evaluate various PPMCC levels in order to choose and arrange various scoring function variables. The results of the tests were finalised by applying the scoring mechanism to each PPMCC level. At last, the ROC curve was used to examine the production scores and find out which PPMCC value had the highest predicting ability.

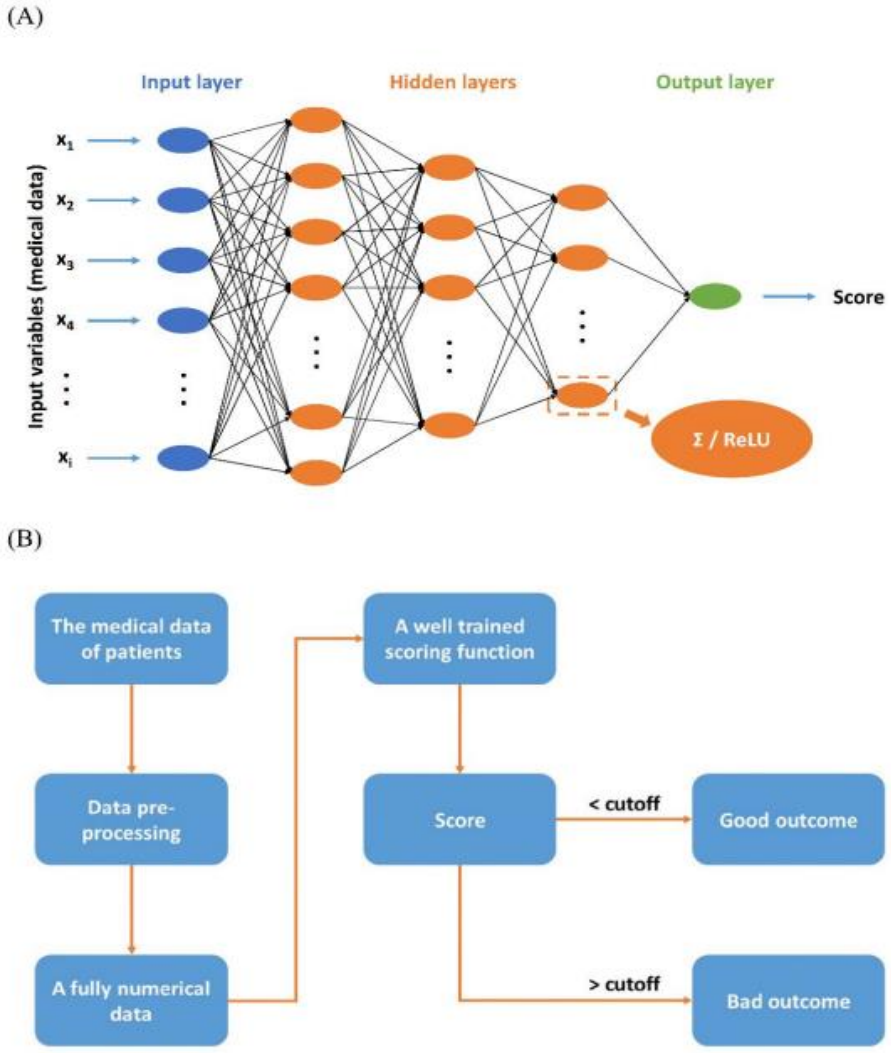


Figure 1:(A) A representation of the multidimensional regression model using deep neural networks for learning. (B) A schematic showing the whole process of the test.

2.5 The Assay Method

See the whole test process in Figure 1B. After undergoing data preprocessing, the 55 patient variables were converted to completely numerical data and scored using a well-trained scoring function, which may include DNN or other ML approaches. Lastly, according to the current medical data, the patient's likelihood of a negative result was significantly

increased if their output score exceeded the cutoff value, which was established by ROC analysis of the scoring function. In such a case, doctors and nurses would think long and hard before administering more therapies.

2.6. Analysing Statistics

The SPSS program, version 15.0 (SPSS®®, Chicago, IL, USA), was used to conduct the statistical analyses. The median (interquartile range, IQR) is used to represent continuous data, whereas proportions are used for categorical variables. The odds ratios (ORs) and 95% confidence intervals (CIs) were computed after categorical variables were compared using either the χ 2 test or Fisher's exact test. Depending on the distributions, the Mann-Whitney U-test or the t-test were used to compare continuous variables.

Methods for Machine Learning

Using R software (version 4.0.3), this study compared a DNN model with six other ML algorithms: k-nearest neighbours (k-NN), support vector machine (SVM), random forest (RF), extreme gradient boost (XGB), Glmnet, and regression tree algorithm (Treebag). Caret, a R package (version 6.0-86), was used to run ML models after hyper-parameters were fine-tuned using five-fold cross-validations of five separate runs. The caret package already has the hyper-parameter settings for these ML algorithms established. For example, the KNN model's k, the RF model's mtry, the SVM model's sigma and cost with the radial basis kernel function, etc. In order to avoid building irrelevant ML models, all features were preselected using the normalised feature significance metric. As a last step in evaluating these models, we computed their F1 scores, accuracy, and AUCs on the test set. By determining the likelihood of death using the best threshold point of the receiver operating characteristic (ROC) curve, the accuracy and F1 score of these models could be computed. Furthermore, in order to compare the models' performances, the values of the Matthews correlation coefficient (MCC) and the Cohen's kappa coefficient were computed. Any p-value less than 0.05 was deemed significant, and all p-values were two-sided.

3. OUTCOME

A total of 2472 newborns were prospectively monitored over the three-year trial period. Of these, 1095 met the inclusion criteria and were analysed as they had encountered clinically suspected sepsis. The training set consisted of 765 patients (or 69.8% of the total) while the test set included 330 patients (or 30.2% of the total). Only 28.5% (n = 312) of infants with clinical suspicions of sepsis actually had confirmed sepsis based on blood cultures; the rest had clinical sepsis based on negative cultures. For at least seven to ten days, or until a subsequent negative blood culture, all of these infants were given a full course of therapeutic antibiotics. On average, these instances of probable sepsis manifested themselves at 19.0 (13.0-39.0) days of life. There was no definitive diagnosis for 101 incidents (9.2%). This cohort's 8.2% in-hospital mortality rate (90 neonates died) was consistent across both sets of data.

3.1. DNN Model Feature Selection

Various PPMCC levels were evaluated as part of the feature selection procedure in order to choose DNN model variables. In order to feed five distinct sets of variables into the DNN model, we first tested five different PPMCC levels. At last, the ROC curve was used for each PPMCC level to examine the DNN model's outputs. The outcomes of optimising feature extraction are shown in Figure 2A,B. Figure 2B displays the greatest area under the curve (AUC) for each of the five PPMCC values over all five DNN model runs.

Table 1: Indicators of the scoring function's effectiveness for assessment

Metric	PPMCC > 0.00	PPMCC > 0.03	PPMCC > 0.05	PPMCC > 0.10	PPMCC > 0.15
Area under ROC curve (AUC)	93.85 ± 0.52%	92.15 ± 2.30%	91.95 ± 3.10%	90.88 ± 1.62%	84.65 ± 2.43%
Sensitivity (True Positive Rate)	86.42 ± 3.05%	82.20 ± 3.10%	83.10 ± 4.75%	81.75 ± 1.70%	80.92 ± 4.25%
Specificity (True Negative Rate)	91.89 ± 3.12%	94.75 ± 2.50%	96.10 ± 1.42%	93.85 ± 2.05%	84.95 ± 4.01%
False-Positive Rate (FPR)	8.11 ± 3.12%	5.25 ± 2.50%	3.90 ± 1.42%	6.15 ± 2.05%	15.05 ± 4.01%
False-Negative Rate (FNR)	13.58 ± 3.05%	17.80 ± 3.10%	16.90 ± 4.75%	18.25 ± 1.70%	19.08 ± 4.25%
Positive Predictive Value	54.30 ± 13.25%	64.55 ± 11.70%	70.80 ± 10.80%	59.10 ± 7.90%	36.45 ±

(PPV)					5.10%
Negative Predictive Value (NPV)	98.62 ± 0.30%	98.15 ± 0.28%	98.25 ± 0.42%	98.10 ± 0.14%	97.95 ± 0.45%
F1 Score	0.68 ± 0.07%	0.71 ± 0.09%	0.76 ± 0.06%	0.68 ± 0.05%	0.47 ± 0.05%
Accuracy	91.75 ± 2.60%	94.10 ± 2.15%	95.30 ± 1.22%	93.25 ± 1.75%	84.75 ± 3.30%

3.2: Efficiency Assessment of the DNN Model

The DNN model was evaluated using nine effectiveness evaluation indices, as shown in Table 1: area under the curve (AUC), specificity, sensitivity, false-positive rate (FPR), recall (PPV), negative predictive value (NPV), F1 score, and accuracy. Among the five PPMCC levels, we discovered that a value greater than 0.05 performed the best across six out of nine effectiveness assessment indices. Consequently, the DNN model and others were built using 27 variables chosen at a level, PPMCC > 0.05.

3.3. Predictors' Position in the Scoring Function for Predictions

Table 3 displays the 27 variables and their weights used in the DNN model (PPMCC > 0.05). Requirement of ventilator support during the beginning of clinical suspected sepsis, feeding conditions, and intravascular volume expansion were the top three most important factors in the DNN significance matrix plot.

3.4. DNN Model's Classification Performance

Using the DNN model, we determined the test set's output scores. The testing set included 330 patients; of them, 302 were newborns who made it to release day, while 28 were not so lucky. The score of neonates who did not survive to be discharged was substantially greater (0.93 vs. 0.04, $p < 0.001$; Figure 3A) compared to those who did survive. With an empirical ROC curve of 0.961 and a fitted ROC curve of 0.951 for the DNN model trained on the testing dataset, we can see that this model can differentiate between neonates who passed away and those who made it to discharge. The sensitivity was 89.29% and the specificity was 95.36% when the DNN model's cutoff value was 0.29.

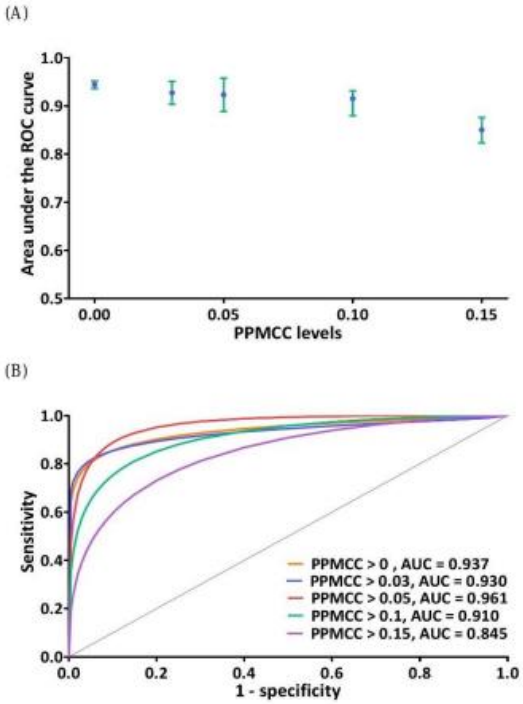


Figure 2: (A) Enhancing feature extraction performance. To fine-tune the feature extraction procedure, we tried out various PPMCC levels to choose various pieces of medical data to use as scoring function variables. The five separate iterations of each scoring function yielded an inaccuracy of one standard deviation. (B) Overall area under the curve (AUC) values for all five scoring functions.The receiver operating characteristic (ROC) and the Pearson product-moment correlation coefficient (PPMCC)

3.5. Evaluations of Different Machine Learning Techniques

Predicting in-hospital mortality was done using the following machine learning algorithms: k-NN, SVM, RF, XGB, Glmnet, and Treebag. The input covariates for all of these methods were the same 27 variables (Figure 4). In terms of the effectiveness of the most accurate single model for outcome prediction, DNN had the highest area under the curve (0.923, 95% CI 0.953-0.893), accuracy (95.64%, 95% CI 96.76-94.52%), F1 score (0.77, 95% CI 0.82-0.72), and MCC value (0.75, 95% CI 0.80-0.70). Furthermore, in order to counteract the impact of the greater Hengda, Cohen's kappa coefficient (Kappa) was used to equalise the precision of the categories. Additionally, out of the seven models we evaluated, the suggested DNN model had the greatest Kappa.

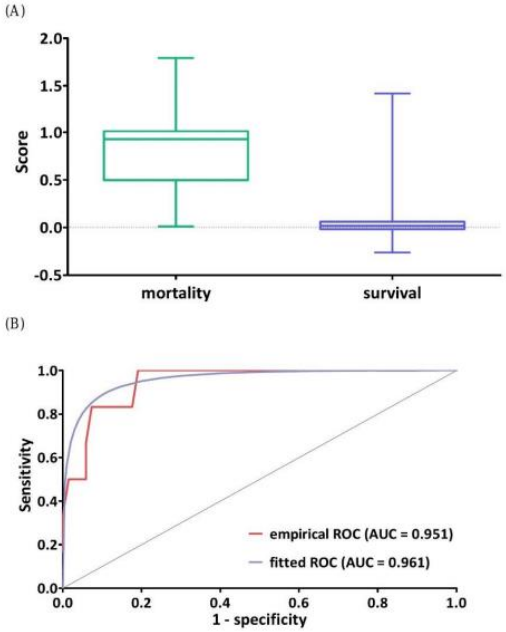
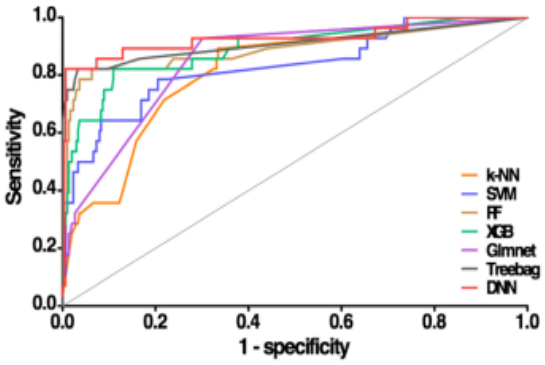


Figure 3: (A) We contrasted the scores of the last 302 survived to those for the 28 individuals passed away beforehand they were released. (B) Analysis of the score's discriminatory power among the death versus control groups using ROC curves. ROA stands for "receiver operating characteristic."



Methods	AUC (95% CI)	Accuracy (95% CI)	Sensitivity (95% CI)	Specificity (95% CI)	F1-score (95% CI)	Kappa (95% CI)	MCC (95% CI)
k-NN	0.745 (0.763 – 0.727)	66.87 % (75.92 % – 57.82 %)	71.43 % (77.14 % – 65.71 %)	66.45 % (77.24 % – 55.65 %)	0.27 (0.30 – 0.24)	0.16 (0.21 – 0.11)	0.23 (0.26 – 0.20)
SVM	0.817 (0.930 – 0.704)	74.75 % (81.54 % – 67.96 %)	73.81 % (87.15 % – 60.47 %)	74.83 % (81.11 % – 68.56 %)	0.34 (0.43 – 0.25)	0.24 (0.35- -0.13)	0.30 (0.42– -0.18)
RF	0.871 (0.914 – 0.828)	94.24 % (97.63 % – 90.85 %)	71.43 % (83.33 % – 59.53 %)	96.36 % (98.81 % – 93.91 %)	0.69 (0.84 – 0.54)	0.52 (0.82 – 0.50)	0.66 (0.82 – 0.50)
XGB	0.874 (0.893 – 0.855)	81.21 % (85.74 % – 76.68 %)	72.62 % (90.79 % – 54.45 %)	82.01 % (88.16 % – 75.86 %)	0.39 (0.40 – 0.38)	0.31 (0.32 – 0.30)	0.37 (0.42 – 0.32)
Glmnet	0.862 (0.874 – 0.850)	78.28 % (83.94 % – 72.62 %)	84.52 % (91.39 % – 77.65 %)	80.80 % (89.55 % – 72.04 %)	0.41 (0.47 – 0.35)	0.32 (0.39 – 0.25)	0.40 (0.45 – 0.35)
Treebag	0.870 (0.942 – 0.798)	95.15 % (97.41 % – 92.89 %)	58.33 % (82.21 % – 34.46 %)	98.56 % (98.74 % – 98.39 %)	0.65 (0.85 – 0.45)	0.63 (0.85 – 0.41)	0.64 (0.84 – 0.44)
DNN	0.923 (0.953 – 0.893)	95.64 % (96.76 % – 94.52 %)	82.86 % (87.51 % – 78.21 %)	96.82 % (98.20 % – 95.44 %)	0.77 (0.82 – 0.72)	0.74 (0.79 – 0.69)	0.75 (0.80 – 0.70)

Figure 4:The median value of the AUC for every version is shown in the bar graph. The greatest efficiency is shown by the red colour. The following acronyms stand for several algorithms: K-NN, RF, SVM, DNN, eXtreme gradient boosting, regression tree method, and Treebag.

4. CONCLUSION

In high-risk neonates with clinically suspected sepsis in the NICU, machine learning (ML) techniques demonstrated strong potential in accurately predicting in-hospital mortality. By analyzing a range of clinical parameters and patient traits, our models were able to identify patterns and predictors associated with poor outcomes. The findings highlight the importance of integrating data-driven tools into neonatal care, particularly for early and precise risk stratification. Certain features, such as abnormal vital signs, laboratory markers, and clinical severity scores, played a significant role in influencing the final outcome. These insights underscore the value of ML in not only supporting clinical decision-making but also in identifying critical indicators that may otherwise be overlooked. Moreover, the ability to continuously update mortality risk in real-time offers a promising avenue for dynamic treatment planning, timely interventions, and resource allocation. While our study demonstrates the feasibility and effectiveness of ML in mortality prediction, it also calls for further research. Future investigations should focus on validating these models in larger, multicentric datasets and exploring how real-time risk adjustment can be practically implemented at the bedside. Overall, ML-based prediction models represent a significant step toward personalized, proactive, and improved care for vulnerable neonates in the NICU.

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