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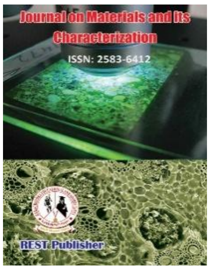

Predicting Electrical Conductivity of Metal Halide and Nitrate Solutions Using Ada Boost Regression: A Machine Learning Approach

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Abstract: *This study investigates the electrical conductivity of metal halide and nitrate solutions as a function of concentration and temperature to improve electrolyte performance in electrochemical applications. Traditional electrolytes pose safety concerns due to flammability and toxicity, thus requiring alternative solutions. The research addresses the knowledge gap in understanding structure-transport relationships in ionic solutions under various conditions. Using a dataset of 100 observations, Ada Boost regression models were developed to predict conductivity behaviour. The results demonstrate strong positive correlations between concentration and conductivity for both halide (r=0.90) and nitrate (r=0.91) systems, with concentration dominating over temperature. The Ada Boost models achieved exceptional predictive accuracy ($R^2>0.98$ for both halide and nitrate conductivity in the experimental data), with minimal error measurements confirming strong generalization. This machine learning approach successfully captures nonlinear ion transport mechanisms, providing a reliable framework for designing optimal electrolyte formulations in advanced battery and super capacitor technologies.*

Keywords: *Ionic Conductivity, Metal Halides, Metal Nitrates, Ada boost Regression, Electrolyte Solutions, Temperature Dependence, Machine Learning Modelling*

1. INTRODUCTION

Conventional electrolytes in batteries and super capacitors pose significant safety and performance concerns, as they are often flammable, corrosive, and highly toxic. This is driving the search for better alternatives. Ionic liquids, especially when combined with metal salts, are gaining importance as next-generation solutions. Their unique characteristics such a large electrochemical stability window, low vapour pressure, good ionic conductivity, and non-flammability, effectively address the limitations of traditional electrolyte solvents. This research focuses on characterizing the electrical conductivity of 1-ethyl-3-methylimidazolium nitrate ([EIm] [NO3]) ionic liquid solutions, examining them in the liquid and gel states with varying concentrations of lithium nitrate salt. The study specifically aims to understand how temperature and salt concentration affect conductivity, thereby assessing the potential of these formulations to act as improved electrolytes [1]. A critical knowledge gap persists in understanding the complex interplay between the ion transport and structure of liquid electrolyte solutions properties at different concentrations and temperatures, which is essential for advancing electrochemical technologies. This study addresses this gap by systematically investigating Aqueous salt solutions' ionic conductivity (κ) containing nitrate ions coupled to various captions, particularly proton, lithium, calcium, and ammonium, as a function of temperature (T) and molar ratio (x). To establish a clear link between structural changes and ionic conductivity, this study combines conductivity measurements with liquid-solid phase diagrams, thereby elucidating the underlying transport mechanisms. This research further evaluates the accuracy of existing predictive equations and a new semi-empirical model that relates both concentration and temperature to conductivity. A key component of this work involves analysing the critical role of activation energy, with the ultimate goal of contributing to a comprehensive phenomenological model for structure and transport in liquid electrolyte solutions [2]. This research seeks to bridge a significant knowledge gap by systematically investigating how the structural properties of liquid electrolytes govern their ion transport mechanisms across a broad range of temperatures and concentrations. The study focuses specifically on aqueous nitrate salt solutions' ionic conductivity (κ) with captions such as proton, lithium, calcium, and ammonium, investigating it as a function of temperature (T) and molar fraction (x). A significant accomplishment of this work is the establishment of a clear correlation between features in liquid-solid Ionic conductivity isotherms and phase diagrams, which provides significant insight into the fundamental mechanisms of ionic transport. Furthermore, this study introduces a new two-variable model that is semi-empirical ($\kappa = f(x, T)$) that accurately fits experimental data, thereby validating existing single-variable equations for conductivity and composition (κ vs. x) and temperature (κ vs. T). This discussion also explores the governing roles of free volume and activation energy, with the combined findings advancing the development of a comprehensive phenomenological model for structure-property relationships in liquid electrolytes [3]. Using mixed-salt electrolytes, combining salts with anions that bind both weakly and firmly provide a viable path toward the development of high-performance, stable batteries. The effectiveness of this approach depends on how the specific salt composition affects the solution structure of the electrolyte. Using With the help of experimental data and classical molecular dynamics simulations, this work demonstrates that the proportion of anions that are weakly (TFSI–) to strongly (NO3–) bound is a critical factor governing ion transport. The findings reveal that this specific ion ratio directly affects both the structural organization and dynamic behaviour of the solution, which together lead to its unique transport properties. This underscores the potential for precisely tuning battery electrolyte properties through strategic anion composition [4]. Structural analysis reveals that all iron (III) complexes adopt a high-spin octahedral geometry, although there are distinct coordination patterns for the anions. In particular, the perchlorate complex contains a dentate perchlorate ion, while there are two monodentate nitrate ions in the nitrate complex. Every anion in the thiocyanate and chloride complexes is synchronized with the metal centre, a property that is partially shared by the bromide complex, in which two bromide ions are coordinated. The thermal behaviour of the complexes of nitrate, thiocyanate, chloride, and bromide, including their phenomena, kinetics, and decomposition aspects, was then investigated using thermo gravimetric and derivative thermo gravimetric techniques [5]. Metal halides exhibit a wide range of chemical behaviour, defined primarily by their ionic and covalent character and varying degrees of Lewis acidity. A clear trend is observed across the periodic table: halides of alkali and alkaline earth metals are predominantly ionic in character, whereas halides of post-transition metals show a more covalent character. This shift toward covalence is accompanied by a significant increase in Lewis acidity for post-transition metal halides compared to their earlier metal counterparts [6]. Guanidinium-based ionic liquids (ILs), particularly those conjugated with trifluorosulfonimide anions, have been studied for their electrochemical properties in two primary contexts: as dye-sensitized solar cells' electrolyte additions and as components in guanidinium-functionalized ion exchange polymer electrolytes. Beyond these bulk electrolyte applications, guanidinium captions and their related salts have also been investigated for their role as redox-functional ligands in metal complexes [7]. Although liquid crystalline phases in ionic liquids generally require cationic species with long alkyl/fluoroalkyl chains or monogenic groups, the use of shorter substituents generally yields non-mesomorph salts. These often form organic ionic plastic crystalline phases. OIPCs represent a rapidly expanding field in materials science and are the subject of intensive research as solid electrolytes valued for their high ionic conductivity in advanced applications [8]. The electrode position of several metals in a variety of deep eutectic solutions has been successfully demonstrated. Under conditions and with brighteners similar to those used in aqueous solutions, these processes yield bright deposits. In particular, for metals such as nickel, cobalt, and zinc, DES-based deposits exhibit enhanced hardness, a property attributed to their unique nanostructure. Furthermore, the specific morphology of the electrode positions has been characterized and is known to critically rely on the type of metal salts dissolved in the DES [9]. Rely on the type of metal salts dissolved in has enabled the electrochemical deposition of metals such as aluminium, a process that previously required temperatures above 100 °C. To improve these applications and foster further research in this field, an important next step is to systematically investigate the connections between ILs' basic characteristics, their molecular structure, and their resulting electrochemical performance [10].

2. MATERIALS AND METHOD

Concentration: Concentration in chemistry quantitatively describes the quantity of solute dissolved in a specific volume of another material (solvent) to create a solution. It is an essential idea for predicting and controlling the behaviour of mixtures in reactions and processes. Common units include molarity (moles of solute per litter of solution), mass/volume percentage, and molality (moles per kilogram of solute). Essentially, it measures the "strength" of a solution. A higher concentration means there are more solute particles in a given space, which directly affects properties such as reaction rate, boiling point, and electrical conductivity.

Temperature: Temperature is a numerical indicator of an object's temperature that is directly correlated with the average kinetic energy of its constituent particles. It's determines the direction of heat transfer, which always flows naturally from a hotter area to a colder one. In terms of science, it is a fundamental parameter in thermodynamics, measured using devices such as thermometers on scales such as Celsius, Fahrenheit, or Kelvin. The latter is an absolute scale, with 0 K representing the theoretical point of zero kinetic energy. Ultimately, temperature is a macroscopic property that reflects the microscopic motion of atoms and molecules.

Conductivity Halide: Conductivity refers to the ability of Fluoride (F^-), chloride (Cl^-), bromide (Br^-), and iodide (I^-) are halide ions to conduct electricity. This occurs when these ions are dissolved in a polar solvent such as water or in a molten, liquid state. In these conditions, the halide ions are mobile and act as charge carriers, moving freely. Conductivity depends on the charge and mobility of the ion; small ions such as F^- have strong hydration spheres in water, which slows them down, sometimes making larger ions such as Cl^- more conductive in aqueous solutions. This principle is fundamental in electrochemistry, where ion mobility facilitates the flow of electricity in batteries, sensors, and industrial electrolysis processes.

Conductivity Nitrate: Conductivity describes the electrical conductivity provided by nitrate ions (NO_3^-) in a solution. As a single covalent ion, the nitrate ion is highly mobile and acts as an efficient charge carrier when dissolved in a polar solvent such as water. This ionic mobility allows a solution of a nitrate salt such as potassium nitrate (KNO_3) to conduct electricity effectively. The concentration of these freely flowing ions directly correlates with conductivity. This property is exploited in various chemical and industrial processes, including use as an electrolyte in electrochemical cells, conductivity standards in laboratory calibration, and in some types of fertilizers where ionic mobility is critical for plant uptake.

Instructions for machine learning: Boosting is a very effective and widely used technique in supervised learning, which works by successively combining a series of simple, weak models to form a single, highly accurate predictive model. This process operates in a greedy manner, with every new student concentrating on the mistakes made by their predecessors. Although its initial conception was for classification, the method has proven to be remarkably versatile across a variety of problem types. A significant and fascinating area of research in this field involves systematically combining boosting algorithms, such as Ada Boost, with well-defined optimization problems. This line of inquiry seeks to provide a deeper theoretical understanding of their computational behaviour and guarantees. As a result, much of the scholarly effort has focused on two primary optimization objectives: maximizing the classification margin and minimizing the exponential loss function, which are central to the algorithm's performance and theoretical foundation.

3. RESULTS AND DISCUSSIONS

This dataset compares the electrical conductivity of metal halide and metal nitrate solutions under varying concentrations and temperatures. The central tendency shows that conductivity increases for both ion species with increasing concentration and temperature, as both factors enhance the number and mobility of charge-carrying ions. However, halide solutions exhibit higher conductivity than nitrate solutions at almost every comparable condition. This performance gap is due to the fact that halide ions (e.g., Cl^-, Br^-) often have higher mobility in solution than the larger, bulkier nitrate (NO_3^-) ion, allowing them to transport electrical charge more efficiently. The relationship is clear: higher conductivity values occur at higher concentrations and temperatures, with halides maintaining a distinct advantage, underscoring the influence of both the ionic species and the physical state of the solution on its conductive properties.

TABLE 1. Descriptive Statistics

	Concentration	Temperature	Conductivity Halide	Conductivity Nitrate
count	100	100	100	100
mean	0.47548	49.8699	75.06467	65.21769
std	0.294472	17.58651	46.96036	40.41154
min	0.015	20.42	2.514	0.01
25%	0.20125	34.5175	37.51075	35.024
50%	0.4695	50.335	66.2855	58.9725
75%	0.73275	65.9725	106.457	91.453
max	0.987	79.14	197.86	167.92

The descriptive statistics in Table 1 allow for seamless integration with various analytical models, as the standardized structure and standard metrics (count, mean, standard) reveal a dataset with strong intrinsic interdependencies. The 100 observations for each parameter (concentration, temperature, conductivity halide, conductivity nitrate) provide a strong foundation. The varying means and standard deviations indicate distinct, well-distributed data ranges, which is important for training models that can operate at different scales. This consistent data profile ensures that predictive algorithms, such as the Ada Boost models evaluated in other tables, are reliably generated and compared, facilitating a unified analytical workflow for comprehensive water quality assessment.

Effect of Process Parameters

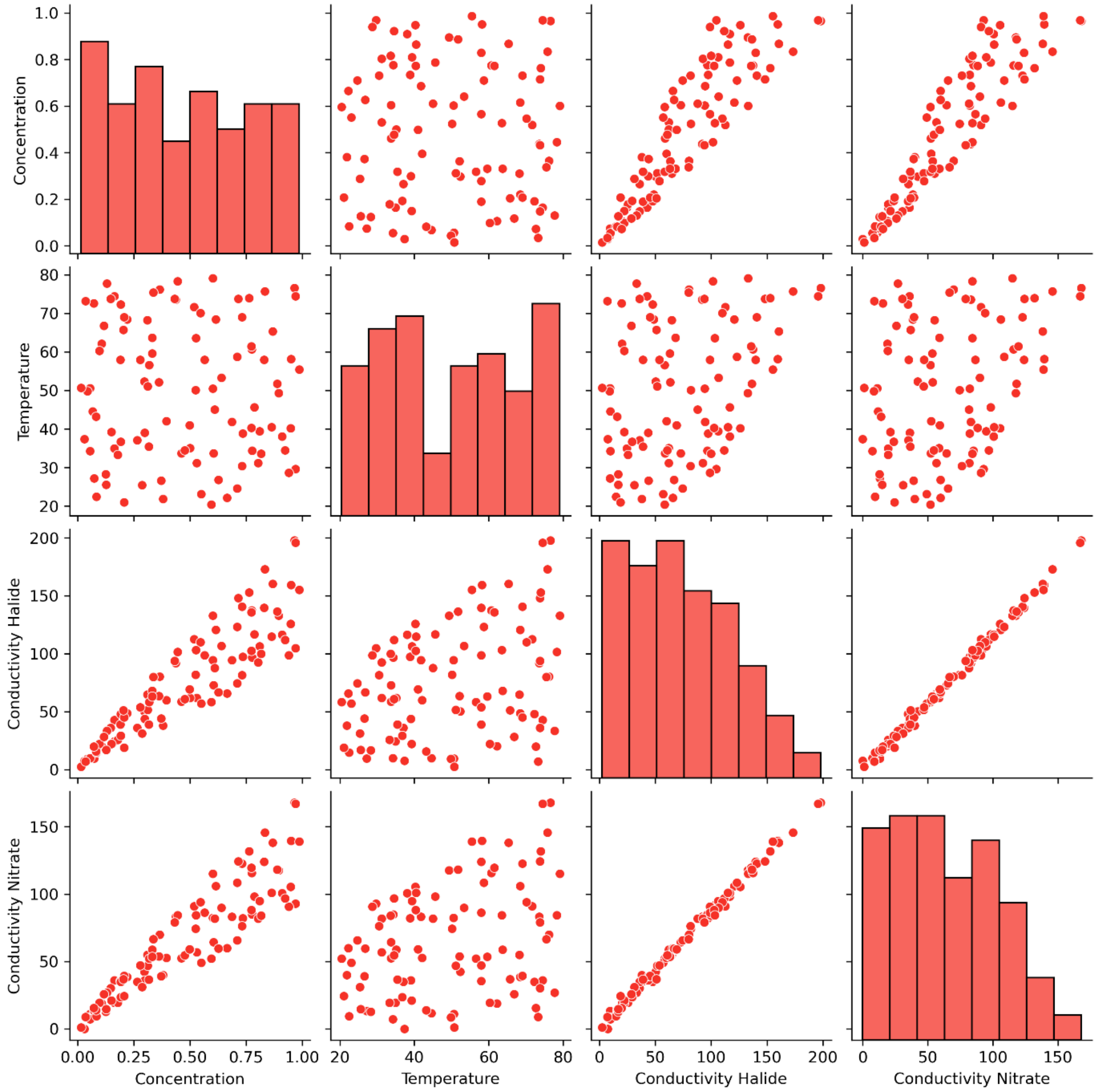

FIGURE 1. Scatter plot of different machine learning-based Conductivity Comparison of Halide and Nitrate Metal Salts

Figure 1 presents scatter plots comparing concentration, temperature, and conductivity for halide and nitrate metal salts using machine learning-based analysis. The plots reveal strong positive correlations between concentration and conductivity for both halide and nitrate salts, while temperature shows a weaker relationship, indicating a dominant influence of concentration on ionic conductivity behaviour.

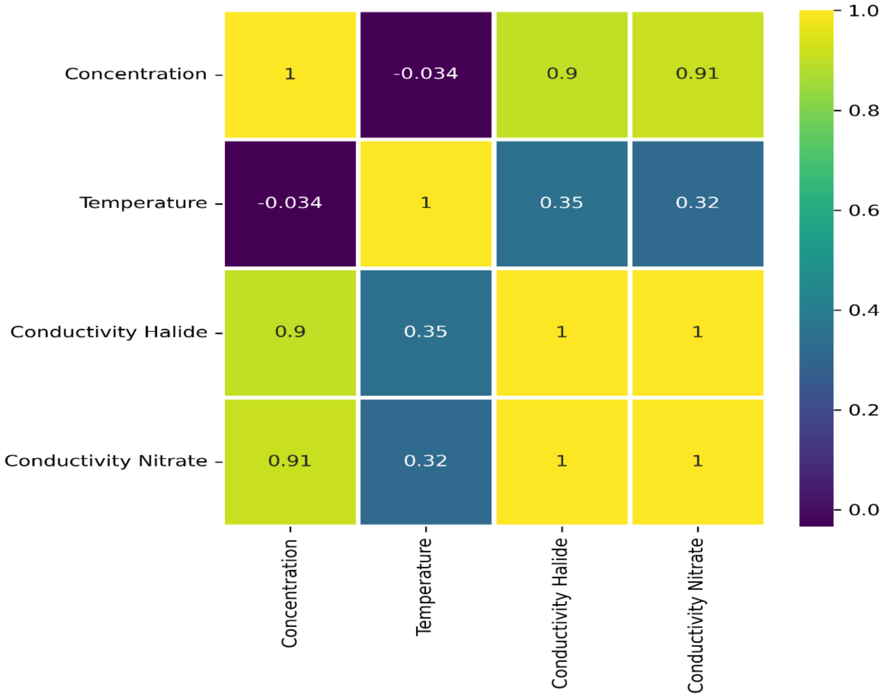

FIGURE 2. Heat map of the relationship between process parameters and outcomes

Figure 2 shows a heat map illustrating the correlations between process parameters and conductivity effects. Concentration shows a strong positive correlation with both halide (0.90) and nitrate (0.91) conductivity, highlighting its dominant influence. Temperature shows a weaker relationship, indicating that conductivity variations are primarily governed by concentration rather than thermal factors in the system studied.

Ada Boost Regression (Conductivity Halide)

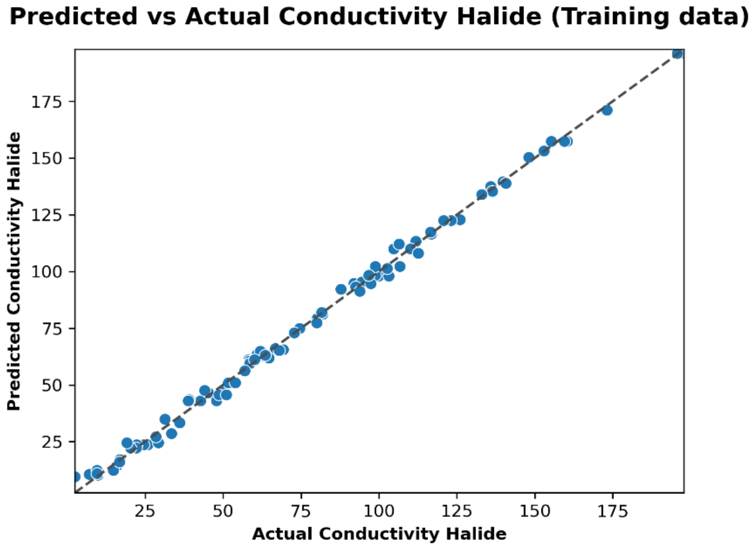

FIGURE 3. Ada Boost Regression on Conductivity Halide: training data

Figure 3 presents the performance of the Ada Boost regression model for halide conductivity using the training data. The close alignment of the data points on the diagonal line indicates high prediction accuracy. The model effectively captures the relationship between the actual and predicted conductivity values, demonstrating its robustness and reliability for modelling halide-based conductivity behaviour.

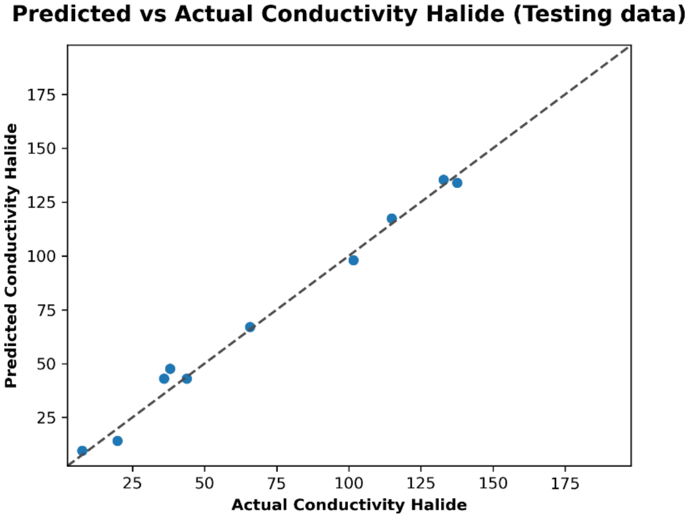

FIGURE 4. Ada Boost Regression on Conductivity Halide: testing data

Figure 4 illustrates the performance of the Ada Boost regression model for halide conductivity on the experimental data. The predicted values closely match the actual measurements on the diagonal line, indicating good generalization. The minimal deviation indicates that the model maintains robust prediction accuracy, effectively capturing the underlying conductivity trends beyond the training dataset.

TABLE 2. Performance Metrics of Ada Boost Regression on Conductivity Halide (Training Data and Testing Data)

Parameter	Data	Symbol	Model	R2	EVS	MSE	RMSE	MAE	MaxError	MSLE	MedAE
Conductivity Halide	Train	ABR	Ada Boost Regression	0.99672	0.99672	7.19586	2.68251	2.14956	7.12767	0.01943	1.91299
	Test	ABR	Ada Boost Regression	0.98932	0.98994	22.25462	4.71748	3.87328	9.70820	0.02303	3.07229

According to Table 2's measurements, the Ada Boost regression model predicting conductivity halide exhibits strong intercorrelation, meaning that it can be reliably integrated into a broader environmental monitoring system. Its exceptional performance on unobserved test data is a key indicator; the high R² (0.98932) and explained variance score (0.98994) confirm its generalizability beyond the training data, capturing the underlying relationship between conductivity and halide concentration with high fidelity. The experimental errors (MSE, RMSE, MAE) are slightly higher compared to the training set – indicating a small expected performance drop – while the consistency in measured error metrics such as MSLE underlines a consistent predictive behaviour. This robustness ensures that the model will provide accurate, reliable outputs when used operationally with other water quality analyses.

Ada Boost Regression (Conductivity Nitrate)

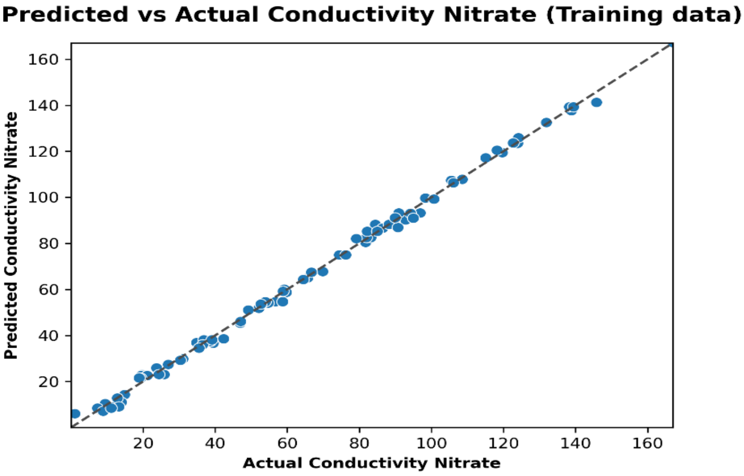

FIGURE 5. Ada Boost Regression on Conductivity Nitrate: training data

Figure 5 shows the training performance of the Ada Boost regression model for nitrate conductivity prediction. The strong alignment of predicted and actual values on the diagonal indicates high model accuracy. The close set of data points demonstrates that the model effectively learns the nonlinear relationships governing nitrate conductivity, ensuring reliable prediction ability.

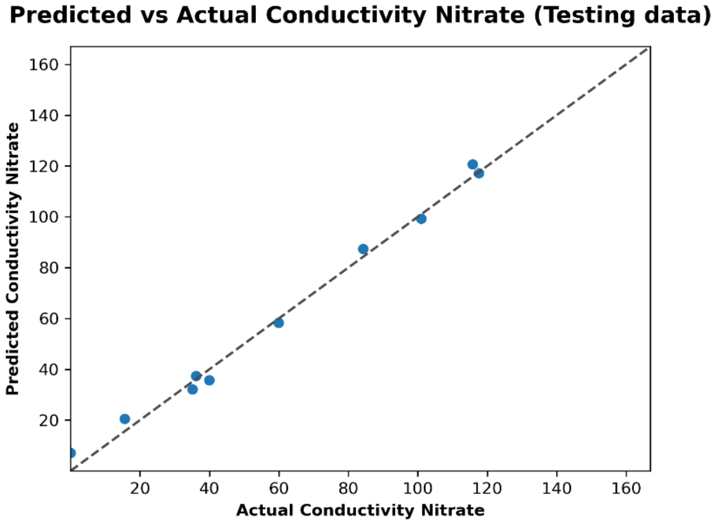

FIGURE 6. Ada Boost Regression on Conductivity Nitrate: testing data

Figure 6 shows the relationship between predicted and actual conductivity nitrate values for the experimental dataset. The points closely follow the diagonal line, indicating that the Ada Boost regression model effectively predicts nitrate conductivity with minimal deviation from the actual measurements.

TABLE 3. Performance Metrics of Ada Boost Regression on Conductivity Nitrate (Training Data and Testing Data)

Parameter	Data	Symbol	Model	R2	EVS	MSE	RMSE	MAE	MaxError	MSLE	MedAE
Conductivity Nitrate	Train	ABR	Ada Boost Regression	0.99761	0.99761	3.86993	1.96722	1.55045	5.08824	0.02377	1.18394
	Test	ABR	Ada Boost Regression	0.99117	0.99187	14.00388	3.74218	3.19445	7.03367	0.43967	3.00443

Based on the performance metrics in Table 3, the Ada Boost Regression model demonstrates exceptional predictive accuracy and strong intercorrelation for predicting conductivity nitrate levels. The performance of this model is consistently strong on both the training and test datasets, which is a key indicator of its generalizability and reliability when applied to different operational environments or integrated with other analytical systems. On the test data, high R^2 (0.99117) and EVS (0.99187) values confirm that over 99% of the target variable's volatility can be explained by the model. Even so, the error measures (MSE, RMSE, MAE) for the test set are higher than those for the training set, this is expected and the difference is not excessive, indicating that the model is not severely over fitting. This balance between high explanatory power and manageable error margins makes the ABR model a suitable and reliable component for interoperable water quality monitoring frameworks.

4. CONCLUSION

This research successfully demonstrates the use of machine learning, specifically Ada Boost Regression, to predict the electrical conductivity of metal halide and nitrate solutions. The findings reveal that concentration dominates ionic conductivity, exhibiting strong positive correlations of 0.90 for halide and 0.91 for nitrate systems, while temperature plays a relatively minor role. Halide solutions consistently show higher conductivity compared to nitrate solutions under comparable conditions, which is due to the higher ionic mobility of halide ions and the bulkier nitrate ions. The Ada Boost Regression models achieved exceptional predictive performance, with R^2 values exceeding 0.98 for both halide and nitrate conductivity predictions on the test data, confirming strong generalization capabilities beyond the training dataset. Minimum error metrics (RMSE, MAE, and MSLE) further confirm the reliability and accuracy of the model in capturing complex nonlinear ion transport mechanisms. These results demonstrate that machine learning approaches can effectively bridge the critical knowledge gap in understanding structure-transport relationships in ionic solutions. The practical implications of this work for advancing electrochemical technologies are significant. The predictive framework developed here provides a reliable tool for designing optimal electrolyte formulations in next-generation batteries and super capacitors, and for addressing the safety and performance limitations of conventional electrolytes. The strong correlation between model predictions and actual measurements ensures seamless integration into broader electrolyte optimization systems. Future research should explore extending this methodology to other ionic systems and investigating additional parameters that affect ion transport properties, ultimately contributing to the development of safe, efficient energy storage technologies.

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