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A Machine Learning Ensemble Approach for Predicting Factors Affecting STEM Students' Future Intention to Enroll in Chemistry-Related Courses

Ardvin Kester S. Ong

School of Industrial Engineering and Engineering Management, Mapúa University, 658 Muralla St., Intramuros, Manila 1002, Philippines; aksong@mapua.edu.ph; Tel.: +63-(2)8-247-5000 (ext. 6202)

Abstract: The need for chemistry-related professionals has been evident with the rise of global issues such as the pandemic and global warming. Studies have indicated how an increase in the amount of professionals should start within the classroom setting, enhancing the interest and motivation of students to pursue higher education in the related field. This study aimed to evaluate and predict factors affecting STEM students' future intention to enroll in chemistry-related courses. Through the use of machine learning algorithms such as a random forest classifier and an artificial neural network, a total of 40,782 datasets were analyzed. Results showed that attitude toward chemistry and perceived behavioral control represent the most influential factors, followed by autonomy and affective behavior. This demonstrated that students' interest, application in real life, and the development of knowledge and skills are key indicators that would lead to a positive future intention for pursuing the course in higher education. This is the first study that has analyzed students' future intentions using a machine learning algorithm ensemble. The methodology and results may be applied and extended among other human factor studies worldwide. Lastly, the presented discussion and analysis may be considered by other universities for their education strategies across different countries.

Keywords: chemistry; machine learning algorithm; random forest classifier; artificial neural network; STEM students; education

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1. Introduction

Chemistry-related courses correspond to the different aspects of applied, social, and life sciences. Graduating from the related courses would develop professionals in the field of medicine, research, academe, government, manufacturing, law, sales and marketing, production, and even business. Ong et al. [1] discussed how sub-disciplines such as analytical, physical, inorganic, biology, and organic chemistry are the five core learnings the students need in order to develop competence. To this end, professionals are needed in different fields [2]. Shwartz et al. [2] and Ong et al. [3] explained how there is a lack of professionals in the different fields of chemistry around the world. Ong et al. [3] explained that this is due to the challenge students perceive when they take on chemistry-related courses.

With the world facing different threats such as global warming and the COVID-19 pandemic, the need for chemistry-related professionals in the field of environmental sciences, medicine, and research is evident. Borges [4] expounded on the need for chemistry-related professionals in different fields. The same research also studied how the connection of a basic knowledge of chemistry in higher education, the development of skills, and support for knowledge are needed to advance the careers of professionals. Supporting this statement, an article from the Nature Editorial [5] stated that a green reset is needed. In accordance, Ong et al. [3] stated that these attributes should start in the classroom, setting up an environment to prepare students to take on the challenges and responsibilities globally. To which end, students should be equipped with the knowledge and skills for this to happen.

From the students' point of view, resistance to taking on the related courses is a challenge. This is why there is a lack of enrollees who consider chemistry-related courses. Previous studies have presented the non-retention and the choice of other educational fields despite the job demand available for chemistry-related professionals [6,7]. Garcia et al. [8] explained how other engineering courses and fields are more desired by STEM student graduates, since chemistry is perceived to be difficult. In response, Ong et al. [3] indicated that several factors, both cognitive and behavioral, should be explored to determine why students opt for other career paths with evident opportunities present.

In Mexico, Hofstein and Mamlok-Naaman [9] concentrated on behavioral factors such as the attitude of students in studying chemistry. However, the results presented how limited information is available to create a thorough discussion on what affects the behavior of students. In the United Kingdom, Burford et al. [10] focused on students choosing neurosurgery—one of the majors which requires several chemistry subjects. Having the option for work–life balance was the most influential factor for students to choose this career path. In Israel, Shwartz et al. [2] considered the behavioral, personal, and environmental factors affecting the career choices of chemistry-related professionals. The results showed that the students' intentions in choosing a career are developed inside the classroom. This was said to be present in how tasks and lectures are being developed. In addition, Ong et al. [3] also presented the same results among students in the Philippines. Their discussion highlighted how the available lessons, their delivery, and their application to real-life scenarios would encourage students to take chemistry-related courses. In addition, cultural differences can affect a student's behavioral and cognitive engagement [11]. Despite the available pieces of literature, the need for exploring behavioral aspects of students to close the gap of understanding why they would choose or avoid chemistry-related courses has been underexplored.

To measure the behavioral aspects of students, an integrated framework of self-determination theory (SDT) and theory of planned behavior (TPB) may be utilized. According to Bunce et al. [12] and Ryan and Deci [13], SDT is a theory usually considered for the education setting. This measures the competency, autonomy, and relatedness of students' motivation [14]. However, other behavioral aspects are not covered in SDT alone. The studies of Ong et al. [3] and Hollett et al. [15] considered integrating TPB to holistically measure the behavior and intentions of students. TPB is a framework used to measure the levels of control that behavior, attitude, and subjective norms of an individual alter their motivation or intention [16]. Guerin and Toland [17] explained how TPB is used in decision-making, covering beliefs from a behavioral perspective. Moreover, Lung-Guang [18] also discussed how these beliefs included either negative or positive engagement. Knauder and Koschmieder [19] then stated that factors such as affect and attitude could measure students' future intentions, in this case choosing chemistry-related courses.

The available studies have mostly utilized multivariate tools such as structural equation modeling (SEM) to measure human behavior [3,19]. Despite SEM being a powerful and reliable tool to determine the causal relationship among latent variables, several studies have criticized the methodology and explored its limitations. Woody [20] discussed how SEM calculates the significance based on the present relationship. Thus, it was explained how the mediating effects of factors may cause the significance level to be lower. Similarly, Fan et al. [21] also stated how the presence of mediators may have low to no significance if the independent variables are far from the dependent variable. To add to this, Duarte and Pinho [22] suggested combining SEM with other tools to validate its findings. Common trends in research nowadays utilize SEM with machine learning algorithms (MLA) such as a random forest classifier (RFC) and an artificial neural network (ANN) [23].

Ong et al. [24,25] considered the utilization of MLAs to evaluate human behavior in the adoption and actual use of technology. It was proven that RFC and ANN can predict factors affecting human behavior with high accuracy. In addition, the studies of Yuduang et al. [23] and Gumasing et al. [26] indicated that the nonlinear relationship of a framework utilized would be viable when analyzed using either ANN or RFC. However, no studies have considered sole machine learning in assessing education-related studies. This study aimed to predict factors affecting senior high school STEM students' intention to enroll in chemistry-related courses utilizing MLAs such as RFC and ANN. Specifically, the main questions this research would want to assess are:

1. What is the most significant factor affecting students' future intentions to enroll in chemistry-related courses among the SDT and TPB latent variables?
2. Will the results of RFC and ANN be consistent with the behavioral analysis in the education setting?

The results of this study may pave the way for the holistic measurement of students' behavior towards their intention, which could be capitalized on by institutions in developing motivations for students. The framework utilized in this study could be applied and extended to measure students' future intentions to enroll in other fields of expertise. In addition, the methodology and results of this study may be considered to evaluate students' behavior in other academic settings worldwide.

2. Conceptual Framework

Presented in Figure 1 is the integrated framework utilized in this study. A total of seven hypotheses were created, with three coming from factors under SDT, autonomy, competency, and relatedness. Under TPB, attitude and perceived behavioral control were considered. In this study, the attitude was separated into two factors under attitude (attitude towards laboratory and attitude towards chemistry subjects) that may affect the affective latent variable. The dependent variable considered is the future intention to enroll in chemistry-related courses.

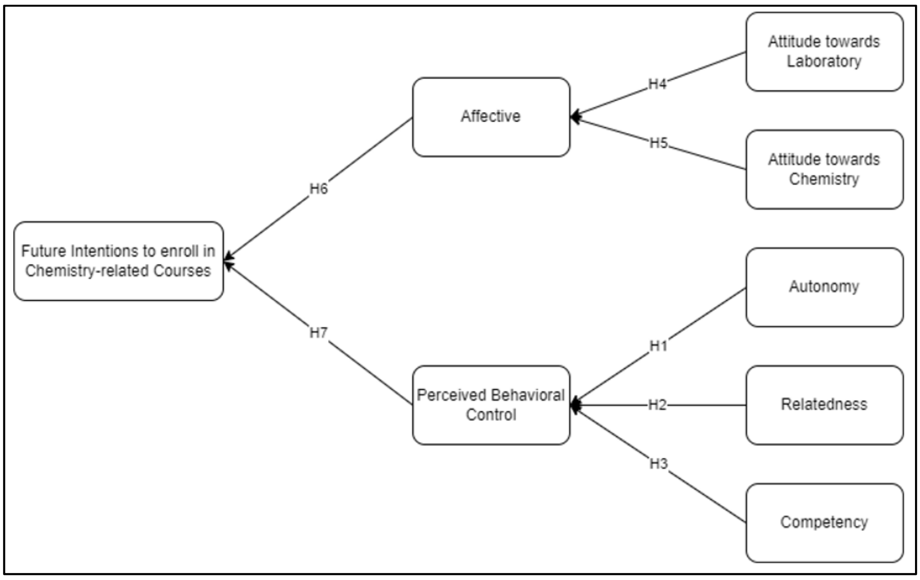

Figure 1. Conceptual framework to measure intention to enroll in chemistry-related courses.

Under SDT, three latent variables are considered following the creation of the theory [13]. Autonomy, relatedness, and competency have been evaluated to measure the behavioral aspects of an individual based on constructs that may be perceived as either negative or positive [3]. Firstly, Hiatt et al. [27] were able to discuss the relationship between autonomy on perceived behavioral control for students who have intentions to enroll for business administration as their form of higher education. Secondly, relatedness is the factor associated with TPB's subjective norm [3], which was disregarded in the educational setting in the early years [28]. However, this factor was seen to be a significant and contributing latent variable that may affect the decision of an individual in the education setting. Lastly, competency is the knowledge and skill required to perform an act without the need for a reward [28]. Students would consider their level of competence to know which intention they would pursue based on their intellectual abilities [29]. It was presented in several studies [3,27–29] how these three latent variables affect the perceived behavioral control that will measure their future intentions either negatively or positively. Thus, the following were hypothesized:

H1. *Autonomy would be the most significant factor affecting students' future intentions to enroll in chemistry-related courses through perceived behavioral control.*

H2. *Relatedness would be the most significant factor affecting students' future intentions to enroll in chemistry-related courses through perceived behavioral control.*

H3. *Competency would be the most significant factor affecting students' future intentions to enroll in chemistry-related courses through perceived behavioral control.*

Attitude may be the negative or positive belief among students about their motivation and intention [18]. In this case, both the attitudes toward the subject and its application in laboratory classes were considered. In chemistry, the theoretical and conceptual aspects are taught in class, while its application is demonstrated in the laboratory [9]. Both the different fields of attitude for students affect their affective behavior, which may have an indirect effect on their future intentions [3]. To engage the measurement of both conceptual and actual applications, it was hypothesized that:

H4. *Attitude towards laboratory would be the most significant factor affecting students' future intentions to enroll in chemistry-related courses through the affective variable.*

H5. *Attitude towards chemistry would be the most significant factor affecting students' future intentions to enroll in chemistry-related courses through the affective variable.*

Affective behavior directly affects an individual's intention, which covers the emotional aspects [30]. The emotional aspect may be affected by the demonstrated attitude of the students and is one of the most important aspects for studying science-related courses [31]. Dicker et al. [32] also highlighted how the affective behavior influenced by students' attitudes would permit a negative or positive effect on their achievements. Several studies by Nwagbo [33] and al Hadid et al. [34] support how affective behavior affects the future intentions of students when dealing with chemistry-related courses. Therefore, it was hypothesized that:

H6. *Affective would be the most significant factor affecting students' future intentions to enroll in chemistry-related courses.*

Perceived behavioral control (PBC) is a person's ability to decide how to act on a matter, either negatively or positively, based on their level of control [35]. Akçayir et al. [31] explored the positive control in behavior among students. It was seen that PBC has a directly proportional effect on future intentions among students upon learning a subject matter. Several studies in an education setting [6,36,37] have proven and justified the effect of PBC on future intentions for career paths, goals, and choices. Thus, it was hypothesized that:

H7. *Perceived behavioral control would be the most significant factor affecting students' future intentions to enroll in chemistry-related courses.*

3. Methodology

3.1. Demographics

The descriptive statistics of the respondents are presented in Table 1. A total of 971 valid responses were collected via convenience sampling during April–June 2022. An online questionnaire adopted from the study of Ong et al. [3] was utilized to evaluate students' future intention to enroll in chemistry-related courses. Only those enrolled in senior high school were considered in this study. The online survey was distributed via Google Forms to different social media platforms to reach senior high school respondents due to the strict COVID-19 protocols and full online learning. Utilizing a 5-point Likert Scale similar to Ong et al. [3], the survey complied with the Data Privacy Act (Republic Act No. 10173) of the Philippines, wherein respondents were asked to fill out and sign a consent form that was approved by the Mapua University Research Ethics Committees (Document No.: FM-RC-22-20). A check box for conformity was obtained from each respondent prior to answering the survey form stating that all information and data obtained would be strictly used for academic research purposes. Upon agreement, respondents would proceed with the survey questionnaire, and those who do not agree would not proceed to answer the survey.

Table 1. Descriptive statistics of respondents (n = 971).

Characteristics	Category	N	%
Age	15	7	0.720
	16	174	17.92
	17	436	44.90
	18	331	34.09
	19	23	2.370
Gender	Male	568	58.50
	Female	401	41.30
	Others	2	0.200
Allowance (in Philippine Peso, PhP)	1000 and below	596	61.38
	Above 1000 and 3000	325	33.47
	Above 3000 and 5000	35	3.600
	Above 5000 and 7000	10	1.030
	Above 7000	5	0.520
Relatives are taking up/took up chemistry-related courses	Yes	164	16.89
	No	807	83.11

From the data gathered, the majority of the respondents were 17 years old (44.9%), 18 years old (34.1%), and 16 years old (17.9%) and were either male (58.5%) or female (41.3%). Following the study of Ong et al. [3], some students in the senior high school level ranged from 15–19 years old (even 20 years old due to acceleration or repetition if the course was not initially completed). The majority have monthly allowances of 1000 PhP and below (61.4%) which is relatively low, followed by monthly allowances of 1001–3000 PhP (33.5%), with the remainder having higher allowances. Lastly, the majority of the respondents do not have relatives who took chemistry-related courses (83.1%) (only 16.9% answered otherwise). With the 42-item constructs and 971 valid responses, a total of 971 $\times$ 42 datasets were considered in this study.

A test for the data collection was conducted for normality using the Shapiro–Wilks Test. The value was within the threshold of ± 1.96, which indicated a normal dataset [3]. It could be noted that several questions such as BC1 and BC2 can be debated to be inclined with control (perceived behavioral control) since Sheldrake et al. [38] explained how the enjoyment in class reflects interest toward the subject matter. Thus, if there is a negative experience (or if students are not enjoying the lesson), they will not be engaged in class. This was therefore included in the control aspect of behaviors in this study. For BC2, Sheldrake et al. [38] also explained how the learning environment of students affects their liking and interest in the lesson or subject matter. In accordance, the common method bias (CMB) using Harman's single factor test was conducted with a threshold of less than 50% [35,39] to determine the applicability of items in their respective variables. The current dataset resulted in 35.02% which indicated that there is no CMB present.

The methodology employed started with the data collection followed by testing its acceptability. Performing data pre-processing adopted from different studies [23,26,39] was conducted. Data normalization and parameter settings for both algorithms were considered.

Thereafter, the validation of the parameters was conducted as an initial optimization with a minimum threshold. Lastly, model creation, choosing best parameters, final model generation, model validation, and interpretation were performed. Figure 2 represents the methodological framework of the study.

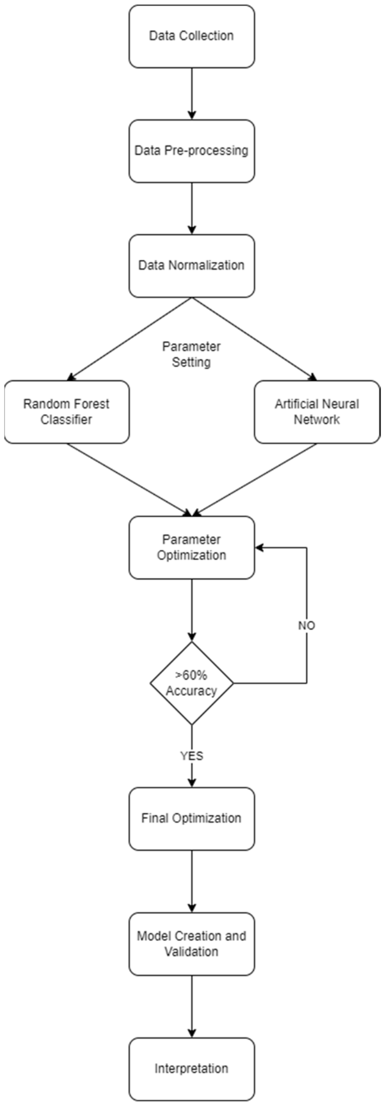

Figure 2. Methodological framework.

3.2. Random Forest Classifier

Random forest classifier (RFC) is a type of machine learning algorithm used for classification. Chen et al. [40] stated how RFC generates a better classification model compared to the normal decision tree, as it generates the best tree with a higher accuracy rate. Ong et al. [24,25] utilized RFC to classify human factors in the adaptation and actual use of an application. It was seen that RFC is one of the best tools to analyze factors influencing decision-making among individuals. In accordance, data cleaning was also utilized in this study using correlation analysis.

A threshold of 0.20 was set for the coefficient, with a 0.05 p-value for acceptance. Following the study of German et al. [35], it was suggested that indicators below 0.20 should be removed since they present little to no significant relationship. Based on the threshold, all indicators were deemed significant ($\geq$0.20)—similar to the study of Gumasing et al. [26]. In light of this, data aggregation through the use of mean values was considered to focus on the latent variables considered. No missing values were observed and no values were dropped in the data pre-processing stage. Lastly, the min–max scalar package was utilized for data normalization. Running the RFC in Python Integrated Development Environment—Spyder 5.0, different parameters were optimized to produce the best tree adopted from studies [24,25,39]. The sklearn package was utilized in the RFC algorithm. Criterion such as entropy or gini, training testing ratios of 60:40 until 90:10, splitters such as random or best, and tree depths from 4 to 7 were considered. With 100 runs per combination, a total of 6400 runs were analyzed in this study.

3.3. Artificial Neural Network

An artificial neural network (ANN) has been utilized nowadays as a hybrid with SEM to classify factors affecting human behavior [23,26]. As a model that mimics how the neurons transfer signals to the brain, studies have concluded that the complex calculation present in this type of MLA can generate more accurate results that would cover the limitations of SEM [24,41]. Yuduang et al. [23] considered a SEM–ANN hybrid to determine factors affecting a mental health mobile application's perceived usability among individuals. It was seen that the results of ANN were able to predict factors affecting human behavior effectively. In addition, Kalinić et al. [42] evaluated consumer satisfaction using ANN. They demonstrated how this type of MLA can determine factors efficiently despite the presence of noise from the dataset and can highlight significant factors despite the non-linear relationship present.

Following the same data pre-processing from RFC, the ANN parameters were also optimized to generate the optimum model. The different activation functions of the hidden layer (tanh, relu, softmax) and output layer (softmax, sigmoid, swish) were considered following several studies [42–44]. In addition, the optimizers (adam, RMSProp, and SGD) were also considered for the optimization process [45–47]. The ANN algorithm was run in this study using Python Integrated Development Environment—Spyder 5.0 with Tensorflow. Keras as the package. Moreover, the class was set to have 5 indicators or normal distribution of the dataset following the 5-point Likert Scale survey response. Similar to other studies [23–26,39], the parameters were adopted from several pieces of literature which were analyzed per combination. With 10 runs per combination (three hidden layer activation functions, three output layer activation functions, and three optimizers), a total of 27,000 iterations (all possible combinations with a division of 10 nodes, until 100 nodes in the hidden layer) were conducted under 150 epochs.

4. Results

4.1. Random Forest Classifier

The results for the RFC from the optimum tree depth (which is five) are presented in Table 2. It could be seen that a 93% accuracy rate with a 0.00 standard deviation was produced using gini as the criterion and best as the splitter. In addition, the precision based on the F1 score presented the highest value of 93.30 and a low standard deviation of 0.823. Utilizing analysis of variance, no significant difference was seen among the results presented. Thus, the highest accuracy with the lowest standard deviation was considered.

The best tree from RFC is presented in Figure 3. It could be seen that attitude towards chemistry (X1) will be the parent node to determine the future intentions of students enrolling in chemistry-related courses. This will then lead to perceived behavioral control (X0). Having a value less than or equal to 2.13 will indicate X0; having values less than or equal to -0.412 will point to X1. If this is not satisfied, this will consider only a high future intention to enroll in chemistry-related courses; otherwise, it will consider autonomy (X2) with a value less than or equal to -0.909, which will lead to very high future intentions to enroll in chemistry-related courses. Nonetheless, if X0 will not be satisfied, it will still consider X0, which will lead to very high future intentions to enroll in chemistry-related courses. If the child node X0 with a value less than or equal to 2.13 will not be satisfied, it will consider X1 and X2, which will lead to high future intentions to enroll in chemistry-related courses.

Table 2. Decision tree mean accuracy (depth = 5).

Category	60:40:00	F1 Score	70:30:00	F1 Score	80:20:00	F1 Score	90:10:00	F1 Score
				Random				
Gini	89.70	90.20	88.00	89.00	89.90	91.00	88.50	89.30
Std. Dev	4.186	3.706	3.469	2.616	3.355	2.261	2.133	2.066
Entropy	91.50	90.67	94.90	96.00	93.40	92.67	93.00	92.50
Std. Dev	3.178	1.936	2.540	1.658	1.561	2.345	2.566	2.587
				Best				
Gini	91.30	92.50	90.12	91.10	93.00	93.30	90.50	91.60
Std. Dev	0.929	1.178	1.037	1.912	0.00	0.823	1.014	1.075
Entropy	92.00	90.56	91.00	90.44	89.93	90.40	89.50	90.20
Std. Dev	0.000	0.527	0.000	0.882	0.00	0.527	0.693	1.302

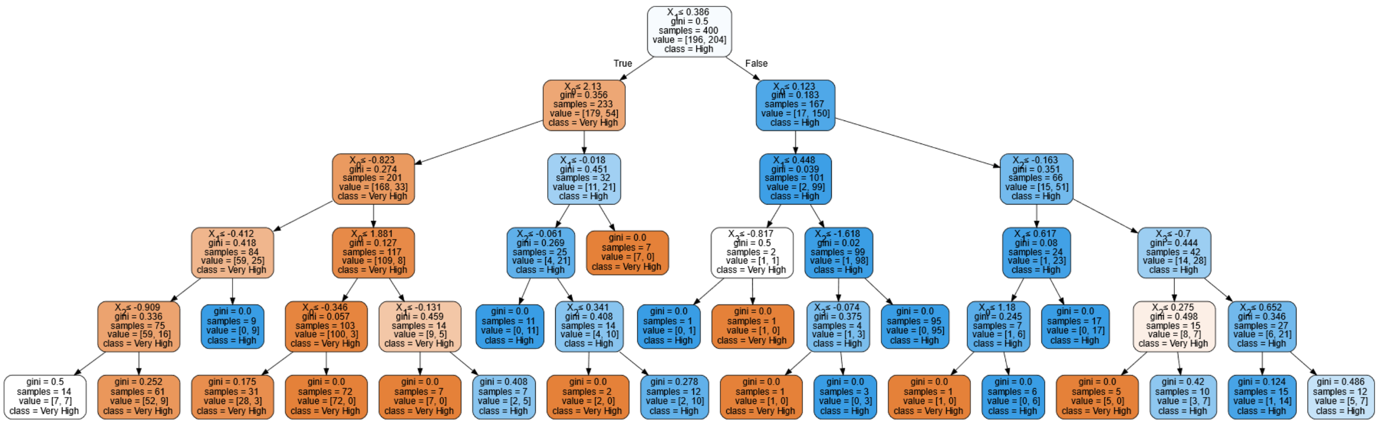

Figure 3. Random Forest Classifier Model. X0—Perceived Behavioral Control (PBC). X1—Attitude towards Chemistry (AC). X2—Autonomy (AU). X3—Affective (AF).

For a child node X0 with a value less than or equal to 0.123, satisfying this will lead to X1 and affective behavior (X3), with a value less than or equal to −0.817. Satisfying this will lead to high future intentions to enroll in chemistry-related courses. If the child node X0 is not satisfied, it will consider X2 with a value less than or equal to −0.163, which will lead to X1 and X0 (this indicates very high future intentions to enroll in chemistry-related courses). Otherwise, it will consider X3 and X2 which will lead to high future intentions to enroll in chemistry-related courses. Therefore, it could be deduced that X1 will be the key indicator for very high future intentions, together with X0. Both X2 and X3 are significant factors as well, which will lead to high future intentions. However, similar to the discussion made by Ong et al. [24,25], only highly significant factors are indicated in the RFC results; thus, there is a need to consider other MLAs such as ANN to identify the most to least significant factor affecting human behavior. In this case, the intent is to elucidate on future intentions to enroll in chemistry-related courses.

4.2. Artificial Neural Network

The result of ANN produced a high accuracy rate of 98.50% with an F1 score of 97.63% for the average precision rate. Presented in Figure 4 is the training and testing validation results for the final run of ANN with 200 epochs. It could be seen that no overfitting was present having the training (blue) and validation (green) loss rates aligned. This indicates the acceptability of the model with no over(under)fitting similar to the findings of other studies [23,26]. To further validate the findings, the precision rate was recorded to be 97.12% and 98% for the recall values. It should be noted that the loss rates may be strikingly identical, but the training loss rate plotting had symbols, which are larger in size. The loss rates are relatively close, but not identical. Following this is Table 3, which represents the average testing and training results of the different latent variables for the initial ANN run.

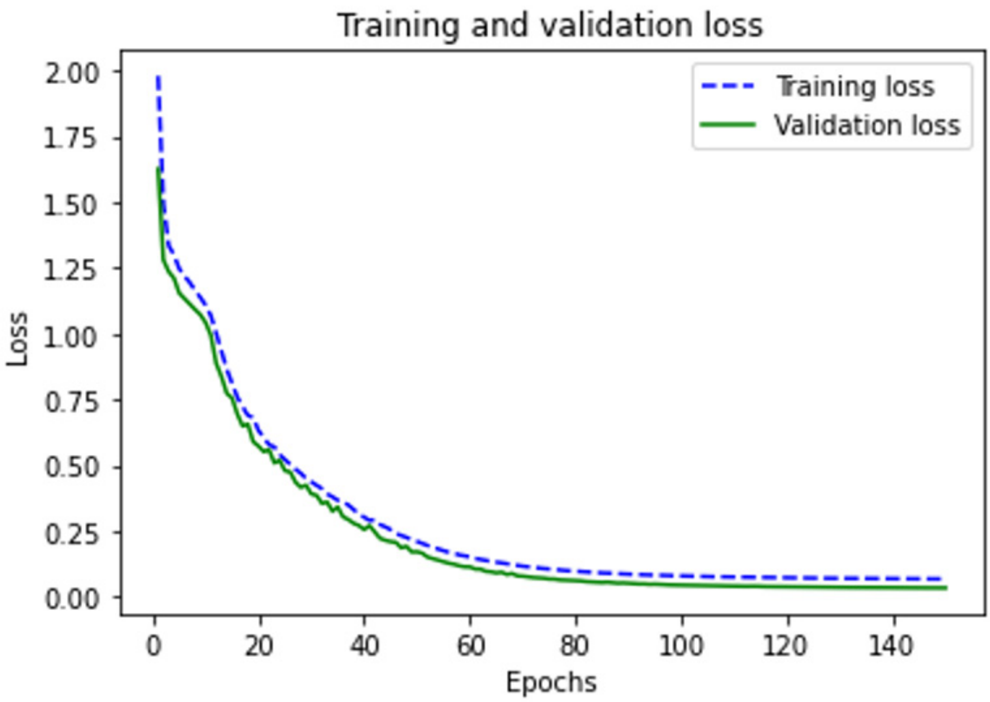

Figure 4. Training and Validation Result.

Table 3. Summary of initial artificial neural network results.

Latent	Average Training	StDev	Average Testing	StDev	F1 Score	StDev
Affective	92.00	4.447	96.41	4.439	95.56	3.210
Attitude Towards Laboratory	80.78	2.108	84.70	3.005	85.97	3.368
Attitude Towards Chemistry	94.25	0.888	98.29	0.784	97.26	1.478
Perceived Behavioral Control	92.51	1.159	98.12	0.294	97.11	1.671
Autonomy	92.43	2.005	96.07	1.651	94.86	2.847
Relatedness	80.21	0.623	85.39	4.440	86.17	3.087
Competency	89.85	1.634	95.90	1.849	94.77	2.898

It could be seen that attitude towards chemistry (AC) gained the highest average testing result, followed by perceived behavioral control (PBC), affective (AF), autonomy (AU), competency (CO), relatedness (RS), and attitude towards laboratory (AL). To verify the results presented, the score of importance was generated as presented in Table 4. Using the optimum parameters of sigmoid for the hidden layer, softmax for the output layer, adam as the optimizer, and an 80:20 training testing ratio, the results in Table 4 are consistent.

Table 4. Score of importance.

Latent	Abbreviations	Importance	Score (%)
Attitude Towards Chemistry	AC	0.180	100
Perceived Behavioral Control	PBC	0.168	93.0
Affective	AF	0.163	90.1
Autonomy	AU	0.144	80.0
Competency	CO	0.134	74.5
Relatedness	RS	0.109	60.3
Attitude Towards Laboratory	AL	0.109	60.3

The Shapley value was utilized in the score calculation of importance. Python Integrated Development Environment—Spyder 5.0 considered in this study followed the SHAP library package with calculations using equation 1. This method was employed since the input variables may change depending on the need of the algorithm. In addition, the generalizability based on calculation would be easier [48]. Karim et al. [49] explained that the SHAP interpretation results in the overall applicability when it comes to the collection of datasets, classifying the contribution and effect of each latent variable in the model. Taking the results into account, each of the variable classifications was deemed to be consistent throughout the analysis. The optimum ANN model is therefore presented in Figure 5.

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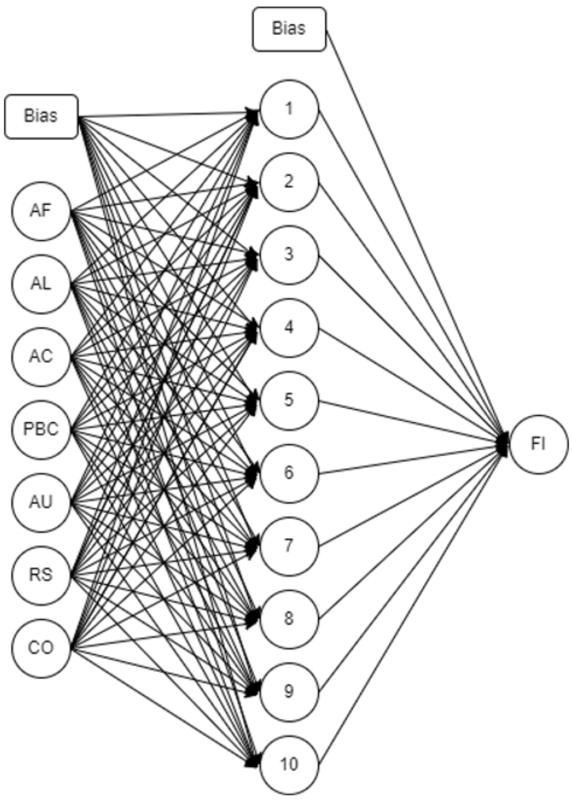

Figure 5. Optimum artificial neural network model. (Left: input layer—latent variables indicated in Table 4; Middle: Hidden layer with number of nodes; Right: Future intention (FI) as the output layer).

In accordance, the test for error rates for both algorithms utilized in this study was conducted. Following the study of German et al. [39], the Taylor diagram (as seen in Figure 6) shows the accuracy rate validation among RFC and ANN. The Taylor diagram was run using Python Integrated Development Environment—Spyder 5.0 with the seaborn package. It was indicated that the Taylor diagram shows the relationship between the accuracy rates with the root mean square error (RMSEA), correlation, and standard deviation [50]. German et al. [39] set the minimum threshold of 20% for RMSEA and 90% for the correlation coefficient. It could be seen from the results that the RMSEA values are less than 20% with consistent factors of latent variable ranking with the RFC and ANN results. Thus, it indicates acceptable and valid results of the machine learning algorithms. All factors were deemed highly significant while both RS and AL were relatively significant.

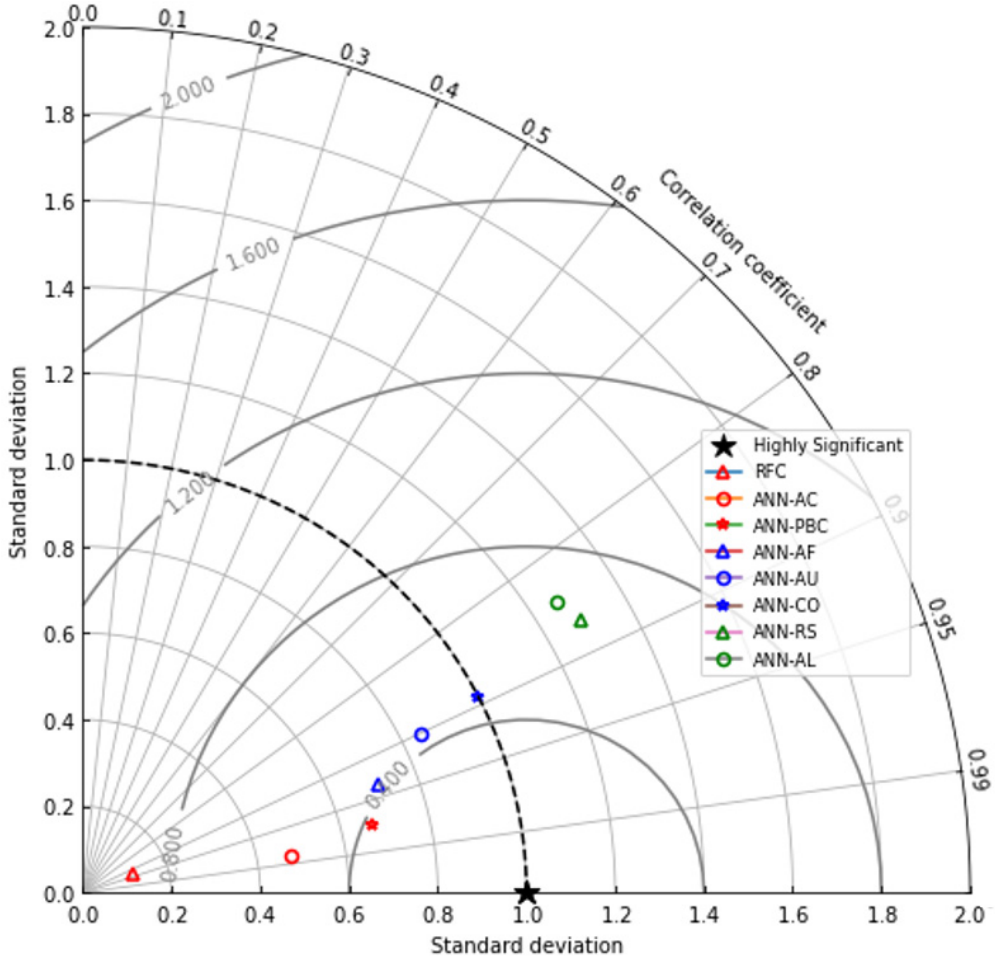

Figure 6. Taylor diagram.

5. Discussion

The results of the machine learning algorithm (MLA) ensemble presented viable and highly-accurate models. The RFC generated a 93% accuracy and the ANN generated a 98.50% accuracy. Ong et al. [24,25] explained and justified that the results for both MLAs would be sufficient in ranking the factors affecting the future intentions of STEM students to enroll in chemistry-related courses. The results showed that AC would be the key indicator for future intentions both from RFC and ANN, followed by PBC, AF, and AU. From the ANN results, competency (CO) was also seen to be significant; however, both relatedness (RS) and attitude towards laboratory (AL) were relatively low with a score of importance that is almost equal to 60%. The threshold was adopted from the study of German et al. [39]. It was explained that compared to forecasting or predicting outputs, there is a 60% more accuracy comparable when using neural network algorithms [51]. Thus, this threshold has been applied by several studies as aligned with significance level which was proven when random forest classifier and neural network results were compared with multivariate tools such as structural equation modeling [24,25,39].

AC would be the most significant indicator in identifying STEM students' future intention to enroll in chemistry-related courses. The indicators showed that students are interested in chemistry to begin with, look forward to chemistry classes, and believe that taking up the STEM strand leads to a more in-depth coverage of chemistry lectures. This presents how the attitude towards a subject matter affects the choices made among students, similar to the study conducted by Dewberry and Jackson [36] from Cyprus. As indicated in the study of Ong et al. [3], students with a positive attitude toward a subject matter in the educational setting would coincide with their decision in their future intentions. Relating to this study, STEM students are observed to have liked chemistry, which leads to having the most significant effect in future intentions. In accordance, it was observed that they have behavioral control over their decision as well.

PBC was shown to have a high significance to future intentions. Students were seen to enjoy chemistry classes, perceive that teachers can explain, apply, and demonstrate concepts to enhance knowledge and skills in chemistry, and have the urge to perform well in chemistry classes. Hagger and Hamilton [52] posited that students who are more interested in a subject matter are more inclined to learn it in a deeper sense. This demonstrates that students would want to pursue the career path due to their interests and how the subject was catered to them. This means that the educator plays a significant role in influencing the intention of students to pursue the course. As explained in the study of Shwartz [2], environmental, behavioral, and personal factors are key indicators for students to pursue the choice in higher education. With the lack of chemistry-related professionals, AC and PBC could be considered for building intentions and motivations by educators to enhance the interests of students in the application of chemistry and its related fields in higher education.

AF was proven to be the third highest significant factor. Students were able to find learning chemistry to be interesting and easy, and would like to learn chemistry deeper. With AF being the emotional aspect of behavior towards something, this positive effect caused a significance trend in the future intentions of students. Masek et al. [53] supported these findings and indicated that when students align their emotions (such as liking a subject matter), they would have a positive intention to pursue this due to interest. However, Hsia et al. [54] explained that even in earlier times, universities have struggled to obtain enrollees for transfer or retention. Thus, it would be beneficial to instill the interest of students at the early stage of learning and continue in the higher level of education. At the same time, their emotional aspects, such as liking chemistry, may be capitalized upon by the university to pursue the same subject in the institution [3].

AU was a significant factor leading to students' wanting to understand chemistry to learn more about the things around them. It was explained that if students are given the chance to take on projects and learn more, they would perceive learning chemistry as being interesting rather than being a choice [3]—which is one of the indicators of AU in this study. In addition, it could be posited that students want to learn chemistry to understand everything around them. It was also seen from the indicators how learning chemistry became a choice in their current state and how students would want to do better in class. When they are eager to learn, then they would consider this for future and higher education [55]. Jayawardena et al. [55] stated that students' predicament in education would lead to positive future intentions. Similarly, different studies [52,56] justified the findings of this study by indicating how a student's choice is based on their interest and liking rather than influenced by others. Lin et al. [57] discussed how at this stage, both in age and education level, students would want to decide on their own for their future career path. It could therefore be deduced that AU is one of the contributing factors affecting the future intention to enroll in chemistry-related courses among STEM students.

CO was seen to be relatively significant among other latent variables. There is a relationship with regards to students' comprehension in learning chemistry, keenness to solve problems, and application of chemistry in a real-life scenario. The difficulty of applying and extending chemistry outside of classes was seen to be the challenge that led to CO being relatively significant. It was observed from the study of Şen et al. [58] that success factors among students consider their grade point average and even whether they obtain a scholarship. However, it was indicated from the study by Ong et al. [3] that when students are comfortable and interested in what they want to learn, they would pursue it in their higher education. Similarly, Su et al. [59] discussed how interest rather than grades, is a key contributor to students' future intentions. These studies present that CO is one of the significant factors, but not the main latent variable for the determination of future intention. Thus, this justifies the relationship of CO as a significant latent variable in this study.

Both RS and AL were seen to be the least significant factors. Based on the indicators, it was seen that the influence of important people around an individual would lead to a high significance of RS. However, as seen in the demographics, only 16.9% of respondents have relatives who pursued chemistry-related courses, while 83.1% have none. This justifies why RS is one of the least significant latent variables, which posits that students are not influenced by other people when taking up chemistry-related courses; rather, it is their own choice, which could indicate sustainability in taking up the course. Hagger et al. [52] indicated that students would continue pursuing the same course when it is their choice rather than if they are influenced. Guerin and Toland [17] also support the findings of this study—how RS is not the most significant factor for students' future intention in the United States.

In addition, AL was seen to be the least significant. Since the students who responded in the online survey experienced three years of online classes, they were not able to conduct laboratory exercises and experiments. This may have hindered the significance of this latent variable. However, there have been online experiments available, but this may not be sufficient which is why AL was seen to be relatively significant. Sneddon and Douglas [60] explained that the influence of the practical application of theoretical lessons would enhance the interest of students in the subject matter. Experiments should be presented and demonstrated as enjoyable, fun, and interesting in order to engage the students and gain their attention. Estriegana et al. [61] also presented the same results and explained how virtual laboratories should possess similar characteristics to obtain students' attention and interest. Due to the abrupt transition from classroom to online learning, universities could not prepare as much for the course works, which led to an average demonstration of laboratory experiments and exercises [62–64].

STEM students' future intention to enroll in chemistry-related courses considered the delivery of lessons and their interest in pursuing this career. Students are deemed interested in applying chemistry to help society as indicated in the AU latent variable, feel belonging as indicated in AC and CO latent variables, and are knowledgeable about the available opportunities in the career paths as indicated in the PBC and AF latent variables. It could be deduced that universities should enhance their chemistry-related programs, encouraging students to pursue the track in their higher education levels. This would eventually create more professionals in the aforementioned field.

5.1. Theoretical and Practical Implications

Based on the results, it could be posited that machine learning algorithms such as RFC and ANN can measure human factors in the education setting. Following the suggestion of Ong et al. [3] and German et al. [25,35], intentions and behavioral factors may be assessed and evaluated utilizing these tools—a substitute for multivariate tools with a higher accuracy rate of classification and prediction. As support, the analysis of Yuduang et al. [23] presented the SEM and neural network analysis of factors affecting mobile application adoption and showcased how the nonlinear relationships may be accurately measured with neural networks than SEM. Moreover, both Woody [20] and Fan et al. [21] explained how the distance of the latent variable to the dependent variable greatly affects their significance. On the other hand, results also indicated how PBC and AC should be considered by universities as part of their education program to enhance the interest and motivation of students in pursuing chemistry-related courses. It could be deduced that students with interest and passion would lead to continuing higher education in the field. Therefore, the framework and construct of this study may be applied and extended to evaluate other areas and courses of education.

In addition, AU and AF showed to be significant factors leading to high future intentions. Thus, universities may consider evaluating students' interests and likes to determine which track best suits the students for higher education. Not only will this help universities to retain students in their respective tracks but will also encourage students to pursue their future career goals. This could therefore be part of the marketing strategy among universities. They could highlight how the effective evaluation of students could lead to the proper alignment of what students are interested in, what courses would be suited, and what career goals are suitable for them. With these, student retention and continuing education may be applied to universities leading to higher marketability and profitability.

5.2. Limitations

Despite the significant findings and contribution both from the results and methodological standpoint, this study still considers several limitations. First, this study only evaluated chemistry-related courses. Future research may consider analyzing other fields of education to generalize the findings of this study. In addition, the extension of another knowledge management [65] may also be analyzed and considered. Second, this study only measured future intentions. It could be extended by analyzing factors affecting students who are currently taking up the course and evaluating their satisfaction, change in behavior, and interest. This would lead to the evaluation of other factors that may be considered as an extension for future intention and motivation. In addition, attitude towards the learning environment may also be analyzed as an extended factor, covering various aspects such as the teacher, lesson plan, provided support, and the like. To further assess the implications of the study, a follow-up analysis of students who answered the survey may be conducted. The determination of students' responses to positive future intentions may be conducted to correlate the findings. Third, the analysis of implications for future intentions may be conducted in other countries since the current study only covered students in private schools in the Philippines. The public school setup and the difference in geographical location, country, and class modality may be analyzed to present the different behavioral factors affecting students' intention to enroll in chemistry-related courses. Lastly, this study only considered RFC and ANN. Despite the high accuracy rate, other machine learning algorithms may be analyzed such as K-Nearest Neighbors, K-Means, or even PSO and Fuzzy C-Means, and Naïve Bayes for clustering and probability-focused assessment of indicators and latent variables.

6. Conclusions

The need for chemistry-related professionals has been evident in the current generation. The need to focus also on environmental fields has been evident nowadays. The assessment of factors affecting future intentions to enroll in chemistry-related courses is needed to determine how students would engage with their chosen career path. This study considered utilizing a machine learning ensemble of random forest classifier and artificial neural networks to measure human behavior among STEM students. Factors under TPB and SDT were evaluated simultaneously to assess future intentions among students.

With 93% accuracy for RFC and 98.5% for ANN, results showed that the main predicament for future intentions would be the attitude of the subject and perceived behavioral control. These two factors would lead to very high significance for students to have a positive response towards their future intention in choosing a course for higher education. It was also seen that affective behavior and autonomy are significant factors that affect future intentions. The results showed that students' interest (AC and AF), enjoyment (PBC), appreciation (AU), and applicability of the subject matter in real-world (CO) would engage them to choose a course, leading to a professional career path based on a positive point of view. These should be considered and capitalized upon by universities to enhance the intentions and behavioral factors of students in choosing chemistry-related courses. It was observed from the indicators that when students understand the subject, its importance, and the influence of teachers on their knowledge and skills, they would likely consider pursuing chemistry-related career paths.

Universities may engage with students in assessing their interests to determine and guide them to their field of passion. Teachers can also consider the findings of this study to help them be engaged in different fields, especially those who are undecided about their future career goals. The framework and methodology utilized in this study may be applied and extended to other studies related to education in different countries. Lastly, the findings and results discussed may be applied by universities across the world.

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