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Performance Assessment of Predictive Models Employing The Optimiser Technique for Explosive Peak Overpressure

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Abstract

In Peninsular Malaysia, elective estimations of blast execution are significant for ensuring entities and assessments directing operations in such fragment regions as mining and building. These models, which are reliant on AI techniques, perform better than conventional methods in terms of higher accuracy and shorter computational time. Some of the effective optimisation techniques currently in use include Levenberg-Marquardt (LM), Bayesian Regularization (BR), and Scaled Conjugate Gradient (SCG) which were observed to yield less accurate and slow computation. This study examines the characteristics of these optimiser techniques to improve regression and optimisation abilities. The research is conducted through data discovery, data examination, data representation, and model generation. Detailed tests were carried out at two locations with plastic explosive (PE4) and Emulex explosives proving that the process works with real data. These findings further highlighted that BR produced better results by comparing its accuracy and computational time with LM and SCG. The BR regression value is 0.99993 and produces a faster processing time. LM also had high accuracy but needed more epochs. SCG had less regressing accuracy than the other two types, but its speed was much faster. When applied to blast performance forecasting, the incorporation of the element expressed by the following factors such as overfitting was addressed, and accurate predictions were made by applying the BR model. The present investigation corroborates the proposition that does not mean inferiority to BR in blast prediction because of high accuracy and practicality. The results can be used to extend the existing body of knowledge regarding the approximation of safer neural networks after determining weights based on Bayesian Regularization to improve performance and accuracy ratios for predictive models of blast outcomes and peak overpressure.

1. Introduction

It is relevant across several industries and fields of engineering and material science to ascertain the techniques and effectiveness of blast resistance, in safety endeavours to reckon the occurrence effect of blast events. The blast pressure performance is the performance of the material under the blast loading which is defined as the force of an explosion or a blast [1-2]. Conversely, blast pressure performance is concerned with the interaction of a substance or structure regarding the force that is applied by a blast [3]. Measures against potential explosion risk are an essential factor in containment, as they concern buildings, automobiles, and various industrial apparatuses. This is done mathematically, physically through experiments in a laboratory, and even through computer simulations since the purpose of the structures is to be strong enough to minimise the major destruction that a blast may cause.

1.1 Tropical Effects Affect Blast Pressure

Tropical regions are 'hot and wet' all year round, as the temperature and humidity remain high for most of the year. It is noteworthy that the blast pressure may be influenced by factors such as corrosion, material degradation, thermal expansion, and humidity in one or more ways and subsequent investigations must take this possibility into consideration [4-5]. Corrosion as well as degradation of materials are part and parcel of the deterioration process that can be highly likely to occur in the case of metals especially when the temperature is high, and the humidity level is high [6]. This could reduce the rigidity and durability of an inclined building in the sense that if an explosion occurs the building could be easily affected. Thermal expansion refers to the process by which an object or the constituent that composes it expands upon being subjected to heat. The tropical climate significantly bears large fluctuations in temperature leading to repeated expansion and contraction that could force onboard materials to stress and crack formation from micro. Secondly, it is a fact that high humidity increases the sensitivity of the explosives and chemicals used in blasting hence the pressure that follows, will also be altered.

Tropical and subtropical regions require an understanding of the blast pressure crucial factors that include the material type, the temperature, and humidity, and the structural design of the building as well [7]. Material type pertains to the constitution of a substance and its capacity to endure different weather conditions. Elevated temperatures accelerate chemical reactions in explosives. However, the humidity factor is determined by atmospheric moisture and can influence the concentrations of flammable gases. A structural design is a design that considers climatic conditions to improve protection against explosions.

Underperform blast pressure in Malaysia's tropical environment can result in several problems, including increased safety risks, higher maintenance costs, and negative ecological effects. Explosions can greatly increase the susceptibility of buildings and industrial facilities, perhaps resulting in harm or structural failure, therefore presenting a more substantial risk to both human life and property. The costs associated with the maintenance and substitution of impaired materials will increase, posing a significant burden on the economy. In addition, below-par detonation can result in severe ecological repercussions, such as the eradication of natural ecosystems and the pollution of air and water sources.

1.2 Prediction Model Using Artificial Intelligence

Blast performance prediction models can be described as data and algorithm-based models that are used to predict how a material or structure will respond to an explosive blast [8]. Using AI in developing this model, it becomes easier to analyse big data, recognise patterns and give precise predictions that are comparatively more accurate than conventional approaches, alongside executing the model at a faster pace and with less complexities [9-10]. It is a fact that most optimisation of prediction models involves the use of supervised machine learning algorithms such as LM, BR, and SCG.

The relationship between explosion pressure and the degree of explosion is crucial and challenging, mainly due to the profound impact that tropical climates have on structures and the materials that are used in buildings. Therefore, it is easy to see that when the concepts of hazardous threats exist, more extensive investigations and constant monitoring and surveillance are imperative to guarantee the safety of structures located in the tropical climate of Malaysia. Thus, the risk can be mitigated, and proper measures need to be taken, in order to maximise the protection of the people and the material assets.

2. Problem Statement

It is quite critical to forecast the outcome of explosive events and predict peak particle velocity accurately since its efficiency has been dependent on industries like mining and construction. The modern challenge is to create reliable models with high accuracy for describing these characteristics, considering the complications emerging due to variations in environmental and operating conditions. The current optimisation methods involved LM, BR, and SCG, have shown poor accuracy as well as computational time. Therefore, it is necessary to investigate complex methods that can mitigate these constraints and improve the accuracy of the forecasts.

BR artificial neural network (ANN) models are widely used in several predictive modelling areas because they provide better accuracy and generalisation than conventional methods. Zhang et al., (2021) have shown that using the Centre Composite Design–Bayesian Regularisation ANN technique enhances explosion risk prediction robustness and computational efficiency during the pre-design of offshore platforms during the preliminary design phase [11]. Analysing a study of the National Fire Protection Association's Standard 68 (NFPA-68) BR ANNs model for vent zones, Shi et al., (2019) showed that their model is far more efficient than the existing ones. This work reveals how BR ANNs can enhance the accuracy of the predictions in intricate correlation for the enhancement of blast performance and the maximum velocity of particles [12].

2.1 Challenges in Specific Scenarios and Environmental Conditions

Despite the strength of the BR ANN models in stochastic environments, they have limitations in certain zones, for instance, the dispersion of volatile clouds in densely populated places. To overcome these limitations, Shi et al., (2019) used the Artificial Bee Colony (ABC) algorithm and BR ANN [12]. The integration of ABC and BR ANN has been developed to provide better accuracy and stability in numerous cases. When coupled with other optimisation techniques, BR increases the possibility of solving the problems associated with the individual models to enable application in a wide range of industries.

2.2 Applications in Real-Time Predictive Modelling

Different fields have pursued the use of Bayesian network models when it comes to dynamic risk analysis and real-time prediction modelling. Li et al., (2022) have applied the Bayesian network model introduced with fuzzy set theory to adequately assess the changeable fire risk of the petrochemical plants thus enhancing the chances of subclassification of fire risk [13]. Analysing gas pipeline failures, Aalirezaei et al., (2023) has applied a dynamic Bayesian network model [14]. Thus, they pointed out the characteristics such as the age and diameter of the trees that dictated the outcomes of these failures. Bayesian models are found to be effective in addressing these challenges since they can apply probabilistic analysis as well as provide a continual update of the predicted results.

In a more recent study, Mohammadi et al., (2023) specified the use of fuzzy Bayesian networks and their application in quantifying the danger of storage containers in given conditions [15]. The researchers have succeeded in determining common factors that affect the development of chemical leakage and pool fire events. These applications stress the applicable aspects of Bayesian methods in such situations and environments. These methodologies are important in matters regarding blast performance prediction together with the ultimate maximum particle velocity estimation.

Concerning BR and incorporation of hybrid models of the performance of blast and predictions as far as peak particle velocity is concerned, it is possible to improve the accuracy and endurance of the models used. These new technologies can be a revolutionary step in making new safety enhancements used in many different industrial areas compared to previous static techniques and require a re-evaluation of safety consequences in real-time mode. The right direction for further development of the predictive models, and their validation in various environmental and operating conditions should become an important goal of further research.

2.3 Training the Neural Networks

LM, BR, and SCG methods are particularly very useful in the training of neural networks. These strategies maximise or minimise weight adjustments that affect the prediction capability of the neural networks. Every type of neural network such as feedforward neural networks, recurrent neural networks, and convolutional neural networks stands out in its traits that fit certain applications. Understanding these training methods is crucial to make correct judgements about when which of them should be used as being perfect for fine-tuning the blast performance prediction.

It is also preferable to compare these methods of training neural networks with similar technologies used in predicting blast performance with classical regression models and physics-based simulations. As opposed to the discussed neural networks that learn from exposure to data patterns, these conventional methods employ sets of mathematical equations and physical laws. In general, it can be stated that enhanced methods, such as LM, enable neural networks to learn faster in more intricate input structures. Therefore, they are endowed with the capability of presenting better and more inclusive predictive estimates in contrast to traditional methods.

The LM algorithm is an improvement of the gradient descent method and the Gauss-Newton algorithm. This protocol is quite useful in small to medium sized networks because it experiences fast convergence rates. BR uses Bayesian probability to alleviate this problem by using a complexity that networks, thereby offering better predictive capacity for other data [16]. The next one, the SCG, is a modification of the conjugate gradient technique that is most suitable for solving large-scale problems. It performs better when compared to the standard method of gradient descent algorithms. These optimisation techniques address different issues that arise when developing and training ANNs, thus improving efficiency and prediction model accuracy.

2.4 Optimisation Method for Neural Networks

This is an attempt to summarize the different optimisation methods that exist for the training of neural networks namely the LM, BR, and SCG. LM performs relatively better regarding velocity and efficiency in environments of up to a moderate number of networks. Cross-validation and BR is used for the reduction of the degree of overfitting helping the model to generalise better. Nonetheless, SCG is more beneficial for large-scale networks since it is more effective in computational processing. The differences in the structure of each of the methods make it ideal for different types of optimisation problems that are usually encountered when training neural networks. The comparative aspect is displayed in Table 1.

Table 1 *Features comparison of three types of neural networks*

Features	LM	BR	SCG
Type	Training algorithm	Training algorithm with regularization	Training algorithm
Method	The concepts of gradient descent and the Gauss-Newton method are combined in its integration [17].	This technique employs Bayesian inference to address the issue of overfitting.	This is an adapted iteration of the conjugate gradient method that has been specifically tailored for training neural networks.
Effective application	This strategy is exceptionally effective for training feedforward neural networks that are relatively small or medium in size [18].	The network's weights are modified to optimise the alignment with the training data and to discourage complexity, leading to enhanced generalisation of unfamiliar data [17-19].	The methodology is an optimisation strategy that improves the efficiency of the conjugate gradient method by applying scaling [18, 20].
Advantages	It is widely renowned for its fast convergence [18]. It is relevant when the neural network has a moderate number of parameters [19].	BR is an effective method for mitigating problems associated with overfitting in various scenarios, and it generally produces more robust models.	It is frequently used to train neural networks on a large scale, especially when the LM approach may be too slow or require a lot of memory [17, 19].

3. Research Methodology

3.1 Experiment Session

The research methodology comprises four distinct phases, including data acquisition phase, data analysis, data modelling and development of the prediction model, as seen in Figure 1. The data acquisition phase involves conducting extensive trials to investigate explosion patterns. Field blast testing is conducted at two specific sites in Malaysia, specifically Kem Kongkoi, Jelebu, Negeri Sembilan and Chua Teong Chai & Sons Quarry, Kangar, Perlis. The testing entails the utilisation of commercially accessible explosives known as Emulex, which are procured from Tenaga Kimia Malaysia Sdn Bhd. Blast parameters are recorded at the end of the experimentation in an intentional blast using apparatuses like the free field pencil probe, the high-speed data acquisition system and the high-speed camera.

In these field test sessions, various field phases have been captured by recording data such as environmental temperature, distance, the type of explosive material, the number of different shapes, weight, and ignition point. In the data analysis phase, the overall aim is to explore simulations with an emphasis on deciphering the detonation pressure of the blast experiment. The improvement of the accuracy of the peak overpressure regression models leads to the use of feature selection techniques. Verification involves cleaning the data scrutinizing it and acquiring the necessary quality and truthfulness of a dataset.

During the data modelling phase, MATLAB tools have been utilised to develop and establish a military explosion's performance predictive model. In the creation of an ANN for a given problem, the input features and the activation function must be selected accordingly. Lastly, the System Development Phase covers the leap from model definition to the design of a system with an accessible and easy-to-understand interface. This technique employs three models of neural networks (LM, BR, and SCG) in MATLAB fitting tool with the best-performing model chosen. The research methodology is employed in the performance of an extensive evaluation of the properties of explosives and indicators of effectiveness under tropical conditions. In fact, Figure 2 below reveals the correlated scientific activities that have a direct association.

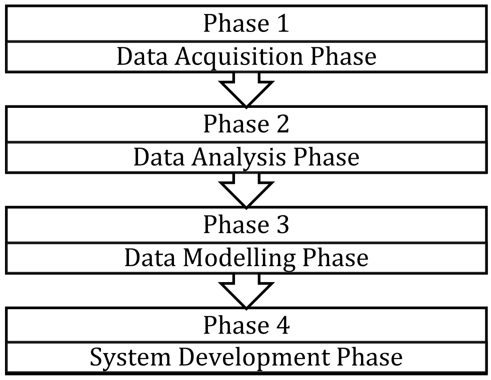

Fig. 1 *Research infographic*

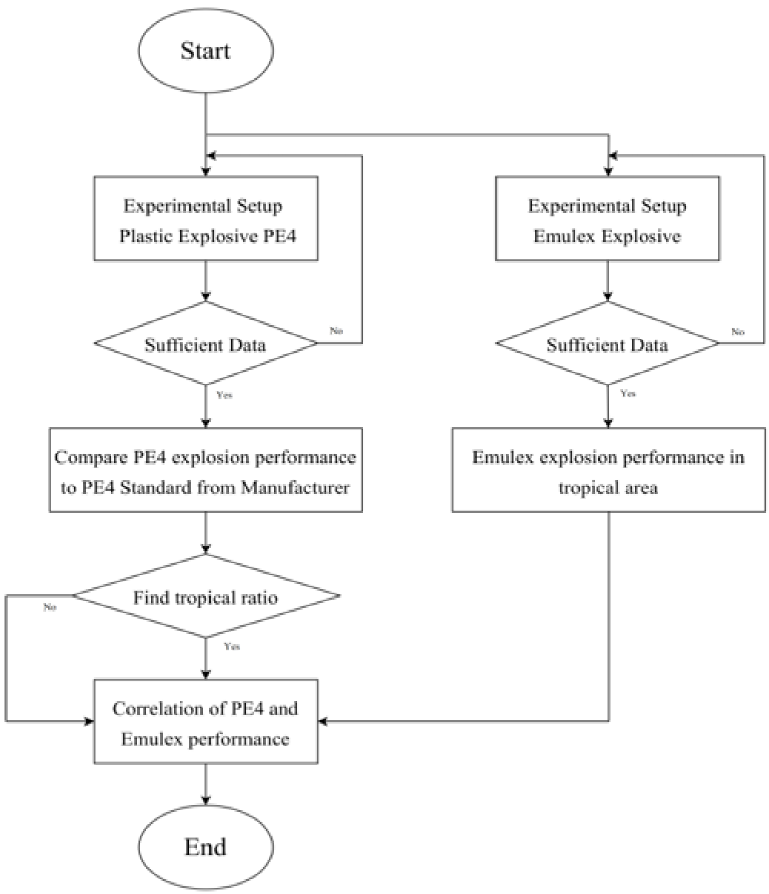

Fig. 2 *Flow chart for the experimental session*

3.2 Data Collection and Pre-Processing

During the study, 144 data sets were collected in the explosion sessions. Thus, from the blast session regarding PE4, there were 72 samples taken while 72 samples from Emulex's blast sessions. By the preprocessing, the 1-100 sessions from the given dataset were used for learning purposes and the 101-144 cycles were excluded from the dataset. The comprehensive list of variables included consisted of a total of seven which was comprised of explosive material, shape mould, distance (meter), ignition point, environment temperature (degree Celsius), weight (in Kilogram), and explosion performance (Mega Pascal), out of which the total data rows submitted were 72. Sets of data were split into 70% for training and 20% for testing via cross-validation. On the other hand, 100 data were used for the training of this network while 22 data were used as sample data. While training the network with the given data, 15% of in each iteration was kept aside for validation. The description of the datasets employed in the study is provided in Table 2 as well.

3.3 Data Partition

The division of the data prepped for the estimation of explosion performance should be different depending on the classification type of the data. As earlier discussed, explosion datasets come equipped with systematic regression data, therefore this structure must be preserved during the training and testing of the model. The research question of this study was to forecast data taking into consideration the previous data that was in it. As a result, if data divisions are not reflected, it may lead to the fact that future information will be a part of the model that predicts the past. Based on the notations made within the framework of the study, the obtained data were divided into sequence distance measurements [21]. By following this process of partitioning, about 70% of the entire data set was set aside for training purposes, while the rest of the 30% was used for the training and validation stage.

Table 2 *Example datasets from experiment sessions*

Explosive material	Shape	Distance, *m*	Temperature, ^{0}C	Weight, *kg*	Ignition Point	Pressure, *MPa*
PE4	Spherical	0.5	30.1	0.5	Top	4.216
PE4	Hemi-spherical	0.5	31.2	0.5	Top	5.209
PE4	Cylinder	0.5	31.4	0.5	Top	5.571
Emulex	Spherical	0.5	34.4	0.5	Top	3.181
Emulex	Hemi-spherical	0.5	34.6	0.5	Top	3.998
Emulex	Cylinder	0.5	31.4	0.5	Top	4.245

3.4 Model Development

Many models including simple classical methods from the machine learning field as well as the more complex ANN algorithms were applied in the framework of the study at hand. As for the machine learning approaches some factors controlled the effectiveness and computational versatility of algorithms that were applied during the model development phase. These parameters are also referred to as "hyperparameters" and relate to the learning process, generalisation, optimisation and complexity. These factors revealed by the study results were the use of regression-based models besides the hyperparameters applied on each model where details are presented in Table 3. As soon as the regression models were built, fitting tools models were built using neural networks to perform fitting [22]. The models have been developed, and the details of hyperparameters are presented in Figure 3.

Though several models were employed, a new model was developed through curve fitting with ANNs. Here, it was inclined to reach the explosion performance results equal to the expected 6 input data in the input layer. Following the input data X1, X2, X3, X4, X5 and X6, a hidden layer of the network should exist, augmented by the output layer that it was supposed to attain. The image of this neural network is illustrated in Figure 3. Table 3 captures details pertaining to activities conducted for the model. It provides the list of datasets used, the proportion of the data used for training and testing, the number of iterations, the optimisation method applied, and other details about the input and output information.

4. Result and Findings

The advantages of using machine learning for the purpose of predicting blast performance are in the fact that the relationships between the parameters that must be considered, and the outcomes can be described by certain mathematical functions with high accuracy. The analysis of the ground vibration experienced in blasting operations is progressively being developed with the employment of machine learning methods. This is an important application because whenever there are movements on the ground, impacts can be transferred to neighbouring regions.

The use of a machine learning algorithm is beneficial for this application because it can capture the non-linear dependencies between the various inputs and the output which include charge weight, distance, and rock properties about the ground vibrations [21-22]. These kinds of relationships are usually not easily discernible and most traditional empirical models fail to capture them while a machine learning algorithm can learn directly from such data. Therefore, this study seeks to analyse the parameters of the optimiser technique responsible for regression performance and enhance its efficiency.

4.1 Evaluation Metrics

To validate the models that were developed following this study, more than one procedure was applied. Metrics such as root mean square error (RMSE) which had been applied when measuring the exactness of statistical prediction models were incorporated in the initial process [23]. The root means square error or (RMSE) was determined by taking the square root of the average of the squared differences between predicted and actual values (Equation (1)).

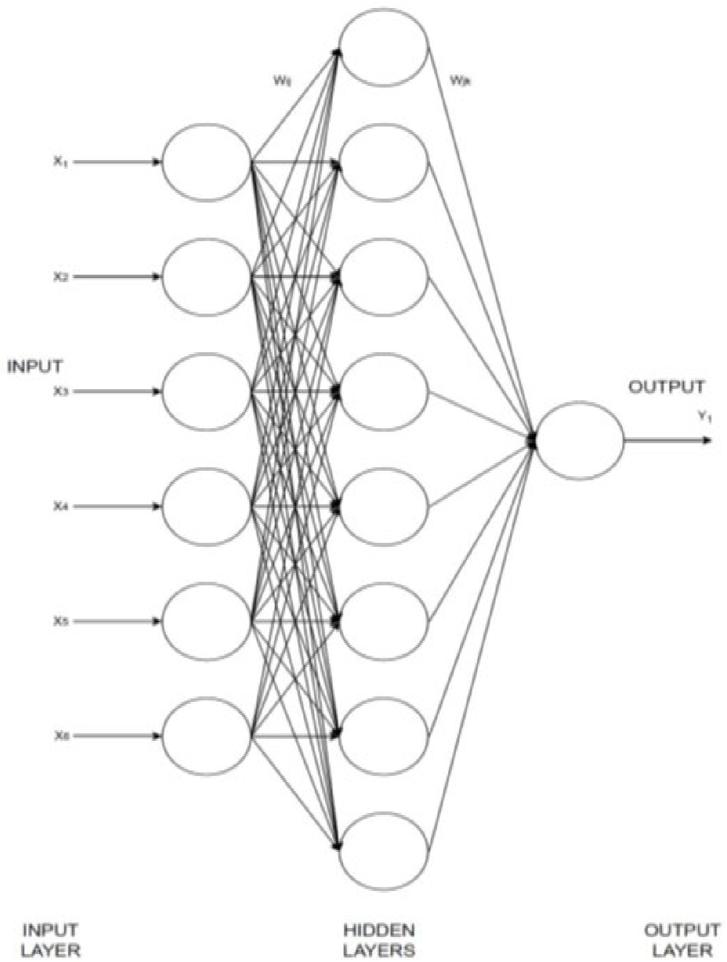

Fig. 3 *The architectural structure of the proposed model*

Table 3 *Training detail information of the model*

Parameters	Value
Dataset	144
Test	15%
Validation	15%
Training	70%
Max Epoch	1000
Optimisation	Bayesian Regularization
Input Data	Explosive material, Shape mould, Distance (m), Ignition point, Environment temperature (°C), Weight (kg)
Output Data	Explosion performance (MPa)
Hidden Layer Size	8
Mu	0.001
Loss Function	Mean square error (MSE)
Number of Fully Connected Layers	1
Activation	Sigmoid

$$RMSE = \sqrt{\sum_{i=1}^{n} \frac{(\hat{a}i - ai)^2}{n}} \quad (1)$$

Sometimes when testing a developed model, it was understood that the RMSE would be low. Higher RMSE indicates that the predicted values were much higher or lower compared to the actual values of blast performance. This example illustrates the lack of effectiveness in finding an accurate model. The formula that gave the lower RMSE value meant that the predicted values were closer to the actual values, which implied that the model was better. Furthermore, MSE results have also been provided with penalties for large errors.

Furthermore, R-squared was employed as the method for the assessment in terms of the framework of the present study. R-squared gives information about the ability of the model to explain the given data and it shows how much of the variance in the dependent variable is explained by the independent variables of the model. Altogether, it was used throughout the entire study to assess the impact of the independent variables on the dependent variable as well as to determine the predictive efficiency of the model.

4.2 Model Analysis

As observed in Figure 3, an effort was made to estimate the explosion performance value in the output layer with 6 input data in the input layer. To optimise this neural network, Bayesian Regularization method was chosen. This optimisation method simply makes sure the network is faster and produces some results. The results that were obtained were found to be rather encouraging. About 15% of cross-validation of the data portion was conducted using random selection and training while testing was performed across 5 clusters. This is a factor enhancing the reliability of training and testing which is an important factor. The training was performed 1000 times, and the results are given in Figure 4.

The training performance of the above model is also represented in the form of a graph depicted in Figure 5. When it comes to the analysis of the given results the major question was how the error rate of the model was reduced gradually. In Figure 5 it was seen that the error rate of the model based on the MSE, and the number of iterations was specifically highlighted.

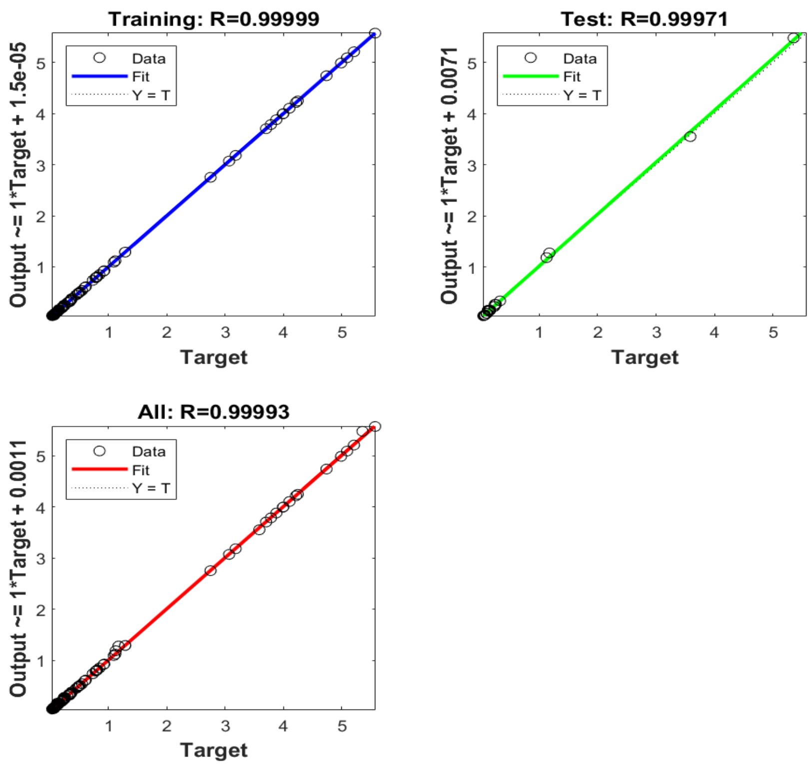

Fig. 4 *Regression plot of BR algorithm*

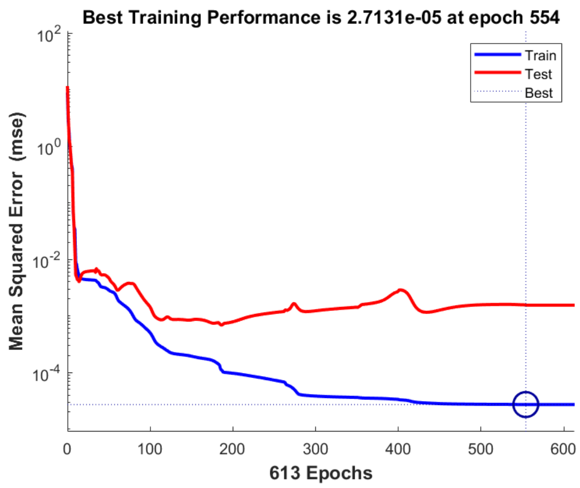

Fig. 5 *Training performance graph of the model*

The hyperparameters were incorporated to yield the best performance in the developed neural network, given in Table 3. In the model implementation, different numbers of hidden layers were used, and it was discovered that the best arrangement was using 3 layers. It contains 1 input layer, 1 hidden layer and 1 output layer. The output layer was the predictive layer. The obtained information includes the corresponding values of the MSE of 0.000027 and regression = 0.999930, which shall be further elaborated in the following section of this paper.

4.3 Result of Predicted Peak Overpressure

This study shows the predictability of peak overpressure via ANN highlights the differences between three diverse types of training algorithms: LM, BR, and SCG. All these algorithms had some distinct features and were characterised by comparable efficacy. There was a good agreement of the LM algorithm to minimise the errors with the regression value of 0.99739 and it successfully trained the dataset as per the direction of intended explosion performance. The identified 20 bins at the end and the error histogram provided additional evidence about the effectiveness of the LM model, revealing 0% error.

Instead, the BR algorithm, which specifically highlights the number of neurons in the initial hidden layer, excelled in Bayesian Regularization and enables a reliable and precise prediction. The resulting regression plot showed an almost perfect regressed input-output relationship with a value of R=0.99993, thus proving the efficient training. The error histogram showed slightly erroneous data (0. 000643) in the middle bin which supports their conclusion of the suitability of the algorithm for explosion performance prediction. However, the analysis also revealed that the training achieved the best accuracy with the aid of the BR algorithm with a faster process time than LM and it took only 554 epochs to get the best training results.

However, the SCG algorithm, though fast, maintained a lower regression value slightly below 1, hence, indicating that the function was still a little off when predicting the output from the input. In the case of the error histogram, the centre bin error was rather low at 0.007496, however, the gradient value was 0.069685, which indicated the difficulties faced in realising the target objective. SCG's convergence at 44 epochs with a validation performance of 0.02523, showed a relatively higher squared mean error indicating that it was less suitable for the explosion dataset than the LM and BR algorithms. All the performance comparisons of the ANN algorithms are summarised in Table 4.

Table 4 *Comparison of the ANN algorithm's performance*

Model Information	LM	BR	SCG
Training	trainlm	trainbr	trainscg
Data division	Random (dividerand)	Random (dividerand)	Random (dividerand)
Training dataset	100 (70%)	100 (70%)	100 (70%)
Testing dataset	22 (15%)	22 (15%)	22 (15%)
Validation dataset	22 (15%)	22 (15%)	22 (15%)
	Progress		
Epochs	16 iterations	613 iterations	50 iterations
Time	00:59 second	05:01 second	00:47 second
	ANN algorithm performance		
Regression	0.997390	0.999930	0.995450
Error at middle bin	-0.009240	0.000643	0.007496
Gradient	0.001993	0.000002	0.069685
Performance MSE	0.023248	0.000027	0.025230
Momentum parameter	0.000100	50000000000	0.069700

5. Summary

From this study, the BR model has been seen to be more appropriate for blast performance forecasting than the LM and SCG models. The evaluation of accuracy and model performance has revealed that BR has the highest accuracy compared to other approaches, making it very suitable for use in estimating employment of this nature. BR could reduce overfitting with Bayesian inference which is a major strength. Combined, it gives outstanding results on the training sets and outperforms competitors, incorporating unfamiliar experimental datasets. Another area that benefits from this system is blast performance prediction, for which the accuracy and consistency of the results obtained are crucial. In this project, the application of Bayesian Regularisation entails employing the optimisation method in tweaking the weights of the neural network. This work adds to the existing knowledge base on how the BR balances and fine-tunes the complexity of the model to offer better accuracy in the prediction of blast outcomes and peak overpressure. Thus, BR is a perfect model for creating accurate predictive modelling in this area of specialisation.

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Conflict of Interest

Authors declare that there is no conflict of interests regarding the publication of the paper.

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Author Contribution

The authors confirm contribution to the paper as follows: ***writing – original draft:*** *Muhamad Izzuddin Abd Rahman, Mohd Sharil Salleh;* ***Methodology:*** *Fakroul Ridzuan Hashim, Mohammed Alias Yusof;* ***Validation:*** *Kamsani Kamal, Muna Saif Humaid Al Rahbi. All authors reviewed the results and approved the final version of the manuscript.*

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