Research on Mechanical Sensitivity Response Prediction of Explosives Based on Machine Learning

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***Abstract*—In order to reduce the workload and uncertainty of conventional mechanical sensitivity tests of explosives, and to obtain the performance parameters of explosives more quickly and accurately, machine learning methods to predict the response values of explosives mechanical sensitivity is proposed. The dataset is constructed by real test, finite element simulation and Monte Carlo data enhancement. By training and hyperparameter tuning for different classification models, we conclude that BP neural network is the best. The model is tested with real test data, and the results show that it is effective and feasible to predict the response values of mechanical sensitivity. It also provides a good reference for multiple QMU (quantification of margins and uncertainties) reliability evaluation of explosives.**

Keywords-machine learning; explosive; safety; QMU evaluation

I. INTRODUCTION

The degree of explosion of explosives under mechanical action is called mechanical sensitivity, including impact sensitivity and friction sensitivity. Bruceton up-down method is widely used in the sensitivity test of products. Due to the limitations of the development period and cost of this method, and the insufficient experimental samples and data required [1], the results are highly stochastic and traditional methods cannot achieve accurate predictions. In recent years, machine learning is uniquely superior in solving nonlinear problems with uncertain inference rules. It has also been applied in the prediction of performance parameters of fire explosives

Reference [2] proposed hessian local linearly embedding (HLLE) algorithm based on SVM. The prediction accuracy of composite explosion parameters exceeds more than 95%. Reference [3] indicated that artificial neural network is obviously superior to multiple linear regression for the prediction of impact sensitivity of compounds. Reference [4] realized the prediction of explosive critical performance based on genetic-neural network with smaller error and better effect.

Back-propagation neural-based genetic algorithm for the calibration of Jones-Wilkins-Lee equal of state parameters of explosive [5] was proposed, the introduction of this method can simplify the optimization process and the test data have proved its high accuracy [6] [7]. Subsequently, the fuel air explosives cloud detonation models can be established.

As few reports on the prediction of the response values of explosives mechanical sensitivity have been seen, this paper combines real test, finite element simulation and Monte Carlo data enhancement [8], builds a suitable machine learning model. The ultimate goal is to input the stimulus amount of impact and friction sensitivities that can quickly and accurately predict the response outcome. This method reduces the amount and consumption of tests and provides a basis for QMU reliability evaluation of explosives.

II. MECHANICAL SENSITIVITY RESPONSE PREDICTION MODEL

A. *Source and construction of the dataset*

Experimental data: According to the national military standard in "GJB772A-1997" (601.2 characteristic drop height method & 602.1 explosion probability method) [9], the determination of impact and friction sensitivity of some kind of explosives are carried out. The impact sensitivity and the logarithmic values of drop height satisfy normal distribution. Giving initial stimulus and step size, and five groups with 125 shots of Bruceton up-down method experiments were performed with falling hammer. The swing hammer of pendulum friction instrument hits the sample of explosives to be measured with the standard pendulum angle and gauge pressure. Two groups with 50 shots of tests were conducted. If the sample is found to be audible, glowing, decomposing and smoking in the above tests, we can judge it as an explosion, i.e, response. The experimental apparatus are shown in Fig. 1.

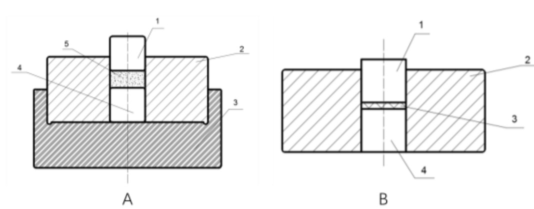

Figure1. Impact sensitivity test (A): 1-Upstroke column, 2-Strike sleeve, 3-Base, 4-Downstroke column, 5-Sample. Friction sensitivity test(B): 1-Upslide column, 2-Sliding sleeve, 3- Sample, 4-Downslide column.

Finite element simulation: ANSYS AUTODYN software was used to simulate the sensitivity tests of explosive particles. Models of drop hammer impacting HMX explosive particles and pendulum impacting slide column were established. Subsequently, we simulated the characteristic drop height method and explosion probability method introduced above. The particle diameters used for the simulation were mixed from 200 to 400 μm. Simulations of the impact sensitivity tests were performed at drop heights of 15.8 to 39.8 *cm* to observe the response results. Simulations of the friction sensitivity tests were conducted with samples actually subjected to pressures of 85-480 *MPa* and pendulum swing angles of 30-90° to observe the reaction degree at different pressures and swing angles. The simulation results are shown in Fig. 2.

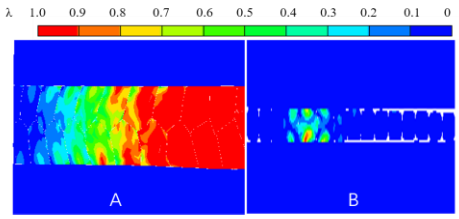

Figure 2. Impact (A) and friction (B) sensitivity simulations, λ means the percentage of response

Monte Carlo simulation data enhancement: The program flow is shown in Fig. 3. The principle of the computer simulation of sensitivity tests is that the program randomly generates a critical stimulus amount and compares it with another group of stimuli generated according to the standard to obtain the response results [8]. In order to expand the dataset of explosive sensitivity tests, Monte Carlo program is written to simulate Bruceton up-down method. μ and σ of the critical stimulus quantities obtained from real tests and simulations as a priori knowledge [10]. Determine the initial stimulus x_1 as μ step size d as σ. Generate long-period normal random numbers x_{ci}~(μ, σ) based on Box-Muller transform. Compare the simulated stimulus x_i with x_{ci}. If x_i is less than x_{ci} , response y_i is noted as 0, x_{i+1} is added to x_i with step d. Conversely, y_i is noted as 1, x_{i+1} is subtracted from x_i by step d. It stops until the sampling number reaches N. An example of the simulation is shown in Fig.4 used by MATLAB.

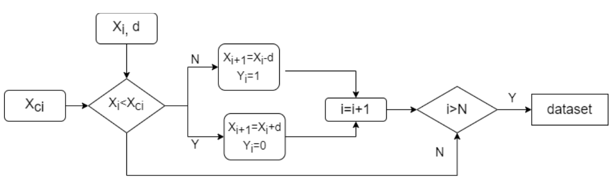

Figure 3. Algorithm of computer simulation up-down method

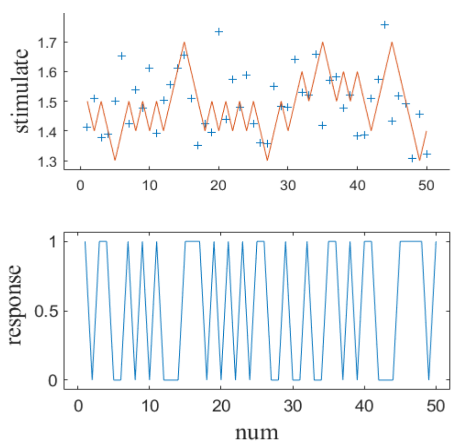

Figure 4. Example of the simulation results

Composition of the dataset: Two parts of the data generated by finite element and Monte Carlo simulation are combined, randomly disrupted and divided into training, validation and test sets. The real sensitivity test data are retained for the final prediction. The composition of the dataset required to train the model is shown in Table I.

TABLE I. COMPOSITION OF THE DATASET

Type	Number of each type			Input	Output
	Real test	Finite element	Monte Carlo		
Impact	125	250	450	Particle diameter, Drop height	Stimulus (0 or 1)
Friction	50	64	190	Particle diameter, Pressure, Pendulum angle	

B. Build model

1) Model training

There are two phenomena in the mechanical sensitivity tests of explosives. We note explosive as 1 and inexplosive as 0. Therefore, the prediction of response values can be considered as a binary classification problem. The following eight classification models are selected:

(A) Fine decision tree. It improves learning efficiency by decision tree pruning, but is sensitive to data noise.

(B) Logistic regression. It has highly interpretative but performances not so good for complex data.

(C) Kernel naive bayes. The generalization effect of limited data is good. However, the input variables should be assumed to be independent of each other.

(D) Quadratic support vector machine. It searches for the maximum margin hyperplane to partition dataset but is sensitive to abnormal data.

(E) Cosine K nearest neighbor. It avoids the problem of sample imbalance according to the majority classification of nearest K samples. But it has high complexity of calculation.

(F) Weighted K nearest neighbor. It makes use of a neighbor weighting function for the purpose of assigning a class to an unclassified sample. But it requires a lot of memory.

(G) Integrated RUS-Boosted tree. It's an ensemble learning method and its performance of processing unbalanced data is relatively robust. But the calculation speed is slow.

(H) BP (back-propagation) neural network. It is composed of input layer, hidden layer and output layer. As it optimizes the model based on the principle of back propagation, it runs faster and has higher accuracy than method (A)-（G）.

The training models adopt 10-fold cross validation. After several hyper-parameter tuning, the training results and model information are obtained as shown in Table II and Table III. The results show that the BP neural network have the best performance.

TABLE II. MODEL OF IMPACT TEST

Model	Accuracy (%)	Precision (%)	Recall (%)	AUC	Training time(s)	Details
A	71.9	72.6	68.6	0.79	1.49	Maximum split: 100; Principle of division: gini impurity
B	71.4	67.9	73.7	0.80	11.21	Loss function: binary cross entropy
C	71.4	70.3	73.7	0.78	9.34	Gaussian kernel
D	71.4	70.3	73.7	0.79	21.48	Quadratic kernel function
E	72.7	77.3	64.5	0.79	0.95	Number of neighbors K=19; Metric: cosine distance
F	73.8	74.5	72.5	0.81	0.73	Number of neighbors K=27; Metric: euclidean distance
G	72.7	69.8	78.6	0.81	5.69	Maximum split: 100; Learning rate:0.1
H	**88.0**	**84.6**	**91.7**	**0.90**	**0.07**	Hidden layers:10; Sigmoid; MSE; Epochs:14; Bayesian regularization

TABLE III. MODEL OF FRICTION TEST

Model	Accuracy (%)	Precision (%)	Recall (%)	AUC	Training time(s)	Details
A	83.9	83.2	88.4	0.88	1.85	Maximum split: 100; Principle of division: Gini impurity
B	71.7	81.8	72.9	0.78	4.10	Loss function: binary cross entropy
C	67.7	86.5	67.4	0.75	5.35	Gaussian kernel
D	80.7	79.7	86.1	0.89	43.26	Quadratic kernel function
E	83.1	87.2	83.1	0.87	46.74	Number of neighbors K=10; Metric: cosine distance
F	84.6	89.8	83.1	0.91	1.05	Number of neighbors K=14; Metric: Euclidean distance
G	85.0	89.9	83.8	0.91	5.51	Maximum split: 40; Learning rate:0.1
H	**88.2**	**91.4**	**91.4**	**0.92**	**0.31**	Hidden layers:30; Sigmoid; MSE; Epochs:62; Bayesian regularization

2) *Prediction of model*

TABLE IV. PREDICT RESULTS

Type	Number of data	Model	Accuracy (%)	Precision (%)	Recall (%)	Binary cross entropy
Impact	125	BP neural network	88.0	90.5	89.3	0.0490
Friction	50	BP neural network	86.0	92.5	90.2	0.0446

Two BP neural network models trained above are selected to predict the response values of the real sensitivity test. Table IV. show that our attempt is effective.

III. APPLICATION OF MODEL IN QMU EVALUATION

A. *The definition of QMU*

Quantification of margins and uncertainties (QMU) method was presented by LNNL and LANL as a creditability evaluation method which can also be used in reliability certification of systems such as high-tech weapons. The mathematical formula of QMU [11] is：

$$Q = \frac{M}{U} \tag{1}$$

$$M = Y_{\text{worst}} - Y_{\text{demand}} \tag{2}$$

M is the best estimate of the margin of the performance parameter and is the subtraction of the worst-case estimate for explosives and the estimate for the lowest requirement (failure criterion). *U* is the uncertainty of *M*. The calculation methods for *M* and *U* are based on specific tests. *Q* is the confidence coefficient, which is used to characterize whether the explosive meets the reliability requirements. The key elements of QMU are shown in Fig. 5.

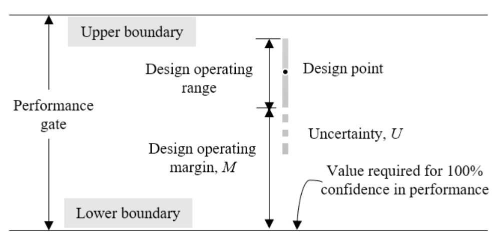

Figure 5. Key elements of QMU

B. *Model prediction and the multiple QMU evaluation*

The QMU method shown above is for single performance parameter. However, the QMU evaluation of mechanical sensitivity of explosives is composed of two parameters including impact and friction sensitivity. We proposed a new multiple QMU evaluation methods based on Euclidean distance of projection curve. The performance curve is shown in Fig. 6. According to the trained model, we predict the response value of sensitivity tests. The model of sensitivity and critical stimulus is established from a large number of predicted values as the performance gate in QMU evaluation system. X_{th} is the performance threshold. X_{PL} is the lower limit of the uncertainty of the performance threshold according to the one-sided confidence interval. X_0 is the safety design value. The Euclidean distance between curves is calculated as margin M and uncertainty U.

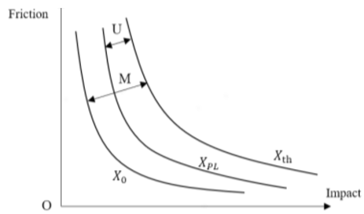

Figure 6. Performance curve of the multiple QMU evaluation

Assume that under the given condition, the safety design value of impact sensitivity is x_1, the one-sided confidence limit is x_2, the critical stimulus is x_3. The safety design value of friction sensitivity is y_1, the one-sided confidence limit is y_2, the critical explosion probability is y_3. This leads to the following equations for the margin and uncertainty in the multiple QMU evaluation method:

$$M=\sqrt{\left(x_3-x_1\right)^2+\left(y_3-y_1\right)^2} \tag{3}$$

$$U=\sqrt{\left(x_3-x_2\right)^2+\left(y_3-y_2\right)^2} \tag{4}$$

M is divided by U as the interval range of Q. If $Q>1$, the uncertainty is included in the margin of performance. We believe that under the given confidence level, the explosive satisfies the reliability requirement that the probability of response does not exceed the safety design value. On the contrary, if there is $Q<1$, the explosive loses its efficiency.

Taking some explosives for example, predict the response values of 25 impact tests and 50 friction tests by the above trained BP neural network. According to the statistics method [12], when the confidence level is 0.9999, the logarithm value of critical stimulus of impact sensitivity is 1.1662, the lower confidence limit is 0.7157, and the safety value is 0.7. The critical explosion probability of friction sensitivity is 0.6920, the lower confidence limit is 0.6039, and the safety value is 0.6. Calculated from (3)(4), the results are shown in Table V. This multiple QMU method can be extended to higher dimensional Euclidean distance for more sensitivity performance parameters.

TABLE V. AN EXAMPLE OF MULTIPLE QMU EVALUATION

	X_{th}	X_{PL}	X_0
Impact	1.1662	0.7157	0.7
Friction	0.6920	0.6039	0.6
Multiple evaluation	$M=\sqrt{\left(1.1662-0.7\right)^2+\left(0.6920-0.6\right)^2}\approx 0.4752$ $U=\sqrt{\left(1.1662-0.7157\right)^2+\left(0.6920-0.6039\right)^2}\approx 0.4590$ $Q=M/U\approx 1.04$		
	Meet reliability requirements.		

IV. COUNCLUSION

According to the results of various model training and prediction, we find that it is feasible to predict the response values of mechanical sensitivity of explosive based on machine learning method. Compared with the conventional sensitivity test method, models of machine learning are faster and have higher accuracy, which can effectively reduce the workload and risk of tests. At the same time, the predicted response values provide an effective reference for the establishment of threshold model of critical explosive sensitivity and multiple QMU evaluation. This research is of great significance to the production, transportation and use of explosives.

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