Application of Support Vector Regression on Neutron Buildup Factors

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ABSTRACT

In this paper the machine learning technique named Support Vector Regression (SVR) method application on neutron buildup factors determination is investigated. When applied on gamma-rays, SVR method shows very good results, leading to the conclusion that there is a potential of using this approach for practical gamma-ray buildup factors determination within established point kernel codes, like QAD-CGCP. A possibility of SVR application on neutron buildup factors estimation has yet to be determined. Neutrons can interact with shielding materials in many ways, including scattering and absorption processes, as well as production of secondary neutrons, protons, gamma-rays or alpha particles. The mentioned by-products can further interact with shielding materials and therefore significantly increase the measured quantity. Additionally produced neutrons can be described with neutron buildup factors. For this study, neutron buildup factors are calculated using approximate formula and are strongly dependent on the shielding material, thickness, and the incident neutron energy range. Typical shielding materials like iron and concrete are observed for neutron energy range 0.5 eV - 14 MeV, and 1 - 10 mean free paths (mfp) thicknesses. Hence, the input vector is multi-dimensional, comprised of the atomic number of the material, shielding thickness, and the incident neutron energy. Output vector is one-dimensional, presenting target buildup factors. Due to high complexity of neutron transport through shielding material, building the SVR model for neutron buildup factor determination is very time and computer hardware demanding. When regarding the size of the training set, one is confronted with a vast number of potential training points. In order to minimize the number of training points and speed up the training process, active learning measures are applied. By combining various active learning methods, the training set is composed of most informative points, leading to good generalization properties of the model with adequate accuracy.

1 INTRODUCTION

The main concern in reactor shielding analysis is attenuation of the fast neutrons and high energy gamma rays which originate not only in the reactor core, but also within the shield itself. Gamma rays are attenuated using heavy materials, like iron or lead and materials containing hydrogen are good neutron absorbers, thus making them effective neutron shields [1]. Therefore, in order to achieve better attenuation effect, practical reactor shields are usually in multi-layer configuration, composed of various materials, including water, lead, iron, aluminium, and concrete in a variety of arrangements.
Reactor shielding calculations are generally performed using either deterministic, Monte Carlo (MC) code, or empirical methods like point kernel and removal diffusion method, depending on the requirements for their accuracy [2]. Empirical methods are used in preliminary design and are characterized by high speed, but at the expense of the accuracy. On the other hand, Monte Carlo calculations perform with high accuracy, but are time and resource consuming. They are usually used in the final studies when precision is of crucial importance. Recently, one of the machine learning techniques, named Support Vector Regression (SVR), was introduced for reactor shielding calculations, specifically for gamma-ray buildup factor estimation [3].

SVR is a relatively new method used for complex classification and regression tasks. It is a kernel based technique, with strong theoretical background in statistical learning theory [4]. The main characteristics of the technique are robustness and good generalization properties. Recent studies have investigated SVR application on gamma ray buildup factors. When applied on gamma rays, SVR shows very good results, leading to the conclusion that there is a potential of using this approach for practical gamma-ray buildup factors determination within established point kernel codes, like QAD-CGGP [3]. The main objective of the present study is to investigate the SVR applicability on neutron buildup factors i.e. to develop SVR model for neutron buildup factor estimation, starting with homogeneous shields, composed of either iron or concrete.

This paper is organized as follows. Support Vector Regression method is presented in Section 2. The methodology of the SVR model development is described in Section 3. In Section 4 results are shown. The paper is summarized up in Section 5.

2 SUPPORT VECTOR REGRESSION

Support Vector Machine (SVM) is a novel machine learning technique used for solving both classification and regression problems. It originated from the statistical learning theory and structural risk minimization developed by Vapnik and Chervonenkis.

SVM is a supervised learning technique, i.e. the model is trained on a set of input/output pairs, typically reflecting functional dependence of the target output ($y$) on the input vector ($\tilde{x}$). The training set is denoted as:

$$D: \{(\tilde{x}_1, y_1), (\tilde{x}_2, y_2), ..., (\tilde{x}_n, y_n)\} \subset \mathbb{R}^n \times \mathbb{R}.$$

Figure 1: SVR using $\varepsilon$ insensitive function

The aim of the modelling is to obtain a function $y = f(\tilde{x})$ which will accurately predict the output value for a new, yet unseen, input value. By "accurately" it is meant that predicted value is within $\varepsilon$ tolerance, as depicted in Figure 1 [5]. In practice one is always confronted with the nonlinear problems as is the case with neutron buildup factor determination. Actually, when dealing with neutrons, high nonlinear properties and multi-dimensional input vector are expected. SVR approach solves the nonlinearity problem by mapping the input vector ($\tilde{x}$) into a higher dimensional feature space $F$. This requires a nonlinear mapping function $\Phi$, and then in this new space a linear regression is conducted. The result of a linear regression is the following linear function:
\[ f(\bar{x}) = \langle \bar{w}, \Phi(x) \rangle + b \]  

where \( \bar{w} \) denotes the weight factor, \( b \) is the bias, \( \Phi(x) \) is the mapping function and \( \langle \bar{w}, \Phi(x) \rangle \) is the dot product in feature space [6]. The estimation of the weight factor \( \bar{w} \) and bias \( b \) is performed using training data. The optimal function \( f(\bar{x}) \), which maximizes the generalization properties of the model, and consequently avoids an "overfitting" effect, is obtained by minimizing a regularized empirical risk:

\[
\min \left\{ \frac{1}{2} \| \bar{w} \|^2 + C \sum_{i=1}^{n} (\xi_i + \xi_i^*) \right\}
\]

subject to

\[
\begin{align*}
y_i - \bar{w} \cdot \Phi(x_i) + b &\leq \varepsilon + \xi_i \\
\bar{w} \cdot \Phi(x_i) + b - y_i &\leq \varepsilon + \xi_i^* \\
\xi_i, \xi_i^* &\geq 0
\end{align*}
\]

where \( \xi_i \) and \( \xi_i^* \) are "slack variables" representing the distance of the training samples from the \( \varepsilon \)-insensitive tube, and \( C \) is a regularization constant which controls the trade-off between the flatness of the function and the tolerance to empirical errors [6].

3 METHODOLOGY

The development of SVR model for neutron buildup factors determination is described in the following subsections.

3.1 Neutron Buildup Factor Determination

The buildup factor is, by its definition, the ratio of the total radiation at any point of interest to the uncollided radiation at the same point [7]. It is applicable to both gamma-rays and neutrons. In simple terms, buildup factor accounts for additional radiation produced by gamma-ray or neutron interaction with matter. Neutrons can interact with shielding materials in many ways, including scattering and absorption processes, as well as production of secondary neutrons, protons, gamma-rays or alpha particles (Figure 2). The mentioned by-products can further interact with shielding materials and therefore significantly increase the measured quantity (flux, fluence or dose rate). Buildup factor is the key parameter for point-kernel approach. Once obtained, buildup factors can be conveniently incorporated into point kernel codes, which then provide solution to the practical problems. Consequently, the accuracy of the desired quantity strongly depends on the accuracy of the buildup factor used in calculations.

Although it is applicable to both gamma-rays and neutrons, the buildup factor concept is widely used only for gamma-ray calculations. Gamma-ray buildup factors for mono-layer shields are calculated and given in a tabulated form, depending on the incident gamma-ray energy, shielding material and thickness. In the case of neutrons, due to high physical complexity of neutron transport through shielding material, buildup factor application in point kernel approach is very limited. Previous investigations have employed MC code for obtaining neutron buildup factors. Also strong effort is made on finding an approximate formula for neutron buildup factors assessment, but former investigations showed that these formulas are applicable only on a limited energy range, shielding thickness and materials.
Abou Mandour and Hassan [8] calculated flux, dose rate and heat deposition buildup factors for fast (14.1 MeV) monoenergetic neutrons and different irradiation geometries using MC code. They also compared the behaviour of neutron buildup factors for different energies and tested the effect of thickness of the medium. Additionally, they provided approximate formulas for buildup factors determination applicable to homogeneous carbon or iron shields and 14.1 MeV neutron energy. Wider energy spectrum was investigated by Shirani and Shahriari [9]. The neutron dose-equivalent buildup factors for lead, iron and water were calculated using MCNP code, covering neutron energy range [0.025-14] MeV and thicknesses ranging from 0.5 to 10 mfp.

The buildup factor estimation for multi-layered shields is more complex than that for homogeneous shields. It depends not only on the present layer, but also on the previously penetrated layer. Abou Mandour and Hassan [10] elaborated on the behaviour of the buildup factor for two-layered shields consisting of iron and carbon. They concluded that buildup factor also depends greatly on the thickness of each layer as well as on the order of materials arranged in the shield. Shin and Ishii [11] introduced simple empirical fitting functions for mono-layer and double-layer shields neutron buildup factors determination. The formulas span neutron energy range up to 400 MeV divided in 12 groups, but are applicable for only two shielding materials, iron and concrete, respectively.

Finally, it is of interest to investigate novel approach, a machine learning technique, named support vector regression, as a possible tool for simple and fast way to determine neutron buildup factors. For this study the above mentioned empirical fitting formula for mono-layer shields is used for obtaining the initial set of neutron buildup factors needed for the learning process. The reason for not using some deterministic or MC code for buildup factor calculation is the fact that both approaches are time consuming, and the primary goal of this paper is just to investigate the possibility of the SVR application, and also to test active learning methodology. More accurate buildup factor determination is forseen in the future work.

### 3.2 SVR Model

As mentioned before, the empirical formula is used to obtain initial set of input/output pairs. Input vector is multi-dimensional, comprised of the atomic number of the material, shielding thickness, and the incident neutron energy. The empirical formula is derived for two different shielding materials, iron and concrete, respectively. Thus in this paper atomic numbers of iron and concrete are observed. It is mentioned that within the formula incident neutron energies up to 400 MeV are included, but in reactor shielding analysis incident neutron energy range from 0.5 eV to 14 MeV is of interest, hence in this paper only this interval is considered. For every neutron energy, the thickness of 1 - 10 mfp is observed. Output vector is one dimensional, representing neutron buildup factor.
Having defined the structure of the input vector and the domain of each component, neutron buildup factor is calculated using the empirical formula and the corresponding coefficients, defined for each energy interval. Once the initial set of points is obtained, the learning process can start. Firstly, it is necessary to define the size of the training and testing sets. Many formulas have been derived to determine the size of the training set. Here $10 \cdot n$ is used, where $n$ is the number of components of the input vector. Since we defined input vector as three-dimensional, hence train set is comprised of 30 points. For testing, two separate sets are defined, validation and evaluation set, respectively. Each of them is composed of randomly selected points and the size of 200 points is chosen arbitrarily. Two separate tests are conducted as a part of the active learning measures introduced in the following subchapter. In each iteration five points are transferred from validation to training set.

Furthermore, recall that incident neutron energy range is from 0.5 eV to 14 MeV and it is divided into eight groups denoted g1 - g8 with neutron energy intervals as follows: [5.49 - 14] MeV, [1.65 - 5.49] MeV, [0.15 - 1.65] MeV, [0.015 - 0.15] MeV, [1.58 \cdot 10^{-3} - 0.015] MeV, [1.01 \cdot 10^{-4} - 1.58 \cdot 10^{-3}] MeV, [1.07 \cdot 10^{-5} - 1.01 \cdot 10^{-4}] MeV, [5 \cdot 10^{-7} - 1.07 \cdot 10^{-5}] MeV. Due to high complexity of the problem under investigation, performed analysis showed that it is best to treat each group separately, i.e. to make an individual model for each group. The models are made using LibSVM within the MATLAB code. LibSVM is an integrated software which provides support vector classification and regression. One of its main features is that it includes interfaces for variety of programs, including MATLAB [12], [13].

Lastly, it is necessary to examine the quality of the developed models. There are many statistical quantities one can use for this purpose. In this paper RMSE (Root Mean Squared Error), RAD (Relative Average Deviation) and $R^2$ are used. This quantities are defined using the following expressions:

\[
RMSE = \sqrt{\frac{\sum_{i=1}^{n}(y_i - f_i)^2}{n}} \quad (3)
\]

\[
RAD = \frac{\sum_{i=1}^{n} \left| \frac{y_i - f_i}{y_i} \right| \times 100\%}{n} \quad (4)
\]

\[
R^2 = 1 - \frac{MSE}{\sigma^2} \quad (5)
\]

\[
\sigma^2 = \frac{\sum_{i=1}^{n} (y_i - \bar{y})^2}{n} \quad (6)
\]

where $y_i$ is the target value, $f_i$ is predicted value, $\sigma^2$ is the variance, representing mean squared deviation. Mean squared deviation is the difference between the target value and the mean target value $\bar{y}$, and $n$ is the total number of points involved in prediction. Generally, the model is more accurate if $RMSE$ and $RAD$ are as small as possible (approaching 0) and $R^2$ is close to 1.

### 3.3 Active Learning Measures

Active learning considers all the measures taken to improve the learning process, i.e. to speed up the learning process and increase accuracy, at the same time requiring a minimal size of the training set [14]. This is achieved by choosing the most informative points for the training set. In the case of neutron buildup factor, as mentioned before, high nonlinearity and the complexity of the problem make the learning process very difficult. Also obtaining initial set of points by more demanding approach using sophisticated deterministic or MC codes would be time and resource consuming. To achieve the desired accuracy, following measures are undertaken:
1. The problem is divided into eight groups according to the energy ranges, and eight separate models are developed.

2. From the initial set evaluation and validation points are selected randomly. Two testing sets are used because in an iterative process that aims to achieve the predefined accuracy of the models, the points that are worst estimated are transferred from validation set to training set. Evaluation set remains unchanged during the learning process.

3. Training points are selected as follows: for the groups that are characterized by strong resonance peaks, training points are selected uniformly near the peaks, in order to obtain better coverage of that part, and the rest of the points are selected randomly.

4. When necessary input data are scaled in the range [-1,1].

Having all the active learning measures defined, the learning process can start following the algorithm depicted in Figure 3.

4 RESULTS

In this section we provide some exemplary results for neutron buildup factors estimation for homogeneous shields comprised of either iron or concrete. We are primarily interested in the quality of the models developed for each energy group based on data obtained by empirical formulas. The dependence of statistical values on the size of the training set for iron and concrete shields is shown in Figure 4 and Figure 5, respectively. In the case of iron shield, groups 1 – 4 required more iterations to reach desired model accuracy. In groups 1 and 2 buildup factors for thick shields are very large, while in groups 3 and 4 relatively low total cross sections result in very thick shields for corresponding mfp thickness due to inversely proportional relationship. Consequently, buildup factor behaviour in groups 1 – 4 is rather complex which asks for a more demanding learning process. Still, by applying different active learning measure, the models ended with desired accuracy with training set size less than 200 points. The other groups achieved the same accuracy in the first iteration (only 30 training points). In the concrete shield case, scaling input data was engaged and the desired accuracy was obtained in the first iteration for all the models. When the scaling
principle was employed for iron shields the improvement of the learning process was not observed.

![Figure 4: Iron shield model quality](image)

![Figure 5: Concrete shield model quality](image)

5 SUMMARY AND CONCLUSIONS

This paper gives a short review of the investigation performed on SVR application in radiation shielding design, specifically in neutron buildup factors estimation. Two types of material are under investigation, iron and concrete, in homogeneous mono-layer configuration. We developed eight individual models in accordance with energy groups for each material. Buildup factors are calculated using approximate formula with corresponding parameters. The obtained results showed good quality of the developed models, measured on different statistical values. Active learning measures applied in this paper led to great simplification of the problem and the desired prediction accuracy was achieved within few iterations. However, additional investigation of the active learning measures is required prior to engagement in the neutron buildup factor model development based on more precise input data obtained by deterministic or MC codes.

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REFERENCES


