Expert Systems With Applications 45 (2016) 161–171

Contents lists available at ScienceDirect

Expert Systems With Applications

journal homepage: www.elsevier.com/locate/eswa

Nonlinear curve fitting to stopping power data using RBF neural networks

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ARTICLE INFO

Keywords:
Radial basis function
Neural network
Curve fitting
Stopping power

ABSTRACT

This paper presents a novel approach for fitting experimental stopping power data to a simple empirical formula. The unknown complex nonlinear stopping power function is approximated by a Radial Basis Function (RBF) neural network with an additional linear neuron. The fitting coefficients are determined by learning algorithms globally. The experiments using the proposed method have been conducted on a benchmark dataset (titanium heat) and a set of stopping power data with implicit noise (MeV projectiles of Li, B, C, O, Al, Si, Ar, Ti and Fe in elemental carbon materials) from high energy physics measurements. The results not only showed the effectiveness of our method but also showed the significant improvement of fitting accuracy over other methods, without increasing computational complexity. The proposed approach allows us to obtain a fast and accurate interpolant that well suits to the situations where no stopping power data exist. It can be used as a standalone method or implemented as a sub-system that can be efficiently embedded in an intelligent system for ion beam analysis techniques.

1. Introduction

In many applications of engineering and science, experimentally measured data are best analyzed by fitting data to an empirical curve or model using nonlinear regression. For example, experimental data on the change in blood pressure of an animal with respect to the drug doses injected are analyzed by fitting them into a curve – the Hill model (a three-parameter logistical equation) and therefore the relevant physicochemical reaction characteristics is determined. The goal of curve fitting is to find a parameterized function that is as close as possible to containing all the data points. Such a parameterized function is also called as a regression curve. It empirically describes the relationship between data and its approximate representation of either an underlying physical process or a real system. The built empirical model is subsequently used to deduce responses of the system, or to predict the data that have yet to be measured. The process of empirical curve fitting often requires a selection of an appropriate functional form (i.e. a parameterized function) or a set of basis functions and a determination of suitable parameters. The selections of an appropriate functional form depend on a good understanding of the underlying science, the observation of data distributions and the properties of the problem. While a list of built-in functional forms, including the logistic, Weibull, and Gompertz, is available in some software packages for nonlinear curve fitting (Crawley, 2007), they or their combinations don't always best describe a complex process in real world applications. On the other hand, determination of fitting parameters can be made by an optimization process over a weighted least-square or non-weighted least-square, in which the sum of the squares between the observed data and those fitted by the model is minimized. If the functional form to be found is linearly dependent on the parameters, the optimization problem of parameters is pretty easy. Nonetheless, when the proposed functional form nonlinearly relies on the unknown parameters (for example, a four-parameter Weibull function), determination of optimal parameters normally needs a lengthy iterative process starting from an initial guess. The initial value largely affects the convergence of the iterative process. Without a good initial guess the iterative procedure may never converge towards a correct solution.

The study of empirical fitting of stopping power data has been germane to many practical applications particularly in material and surface analysis techniques. The stopping process is an energy loss process by which energetic particles are slowed down during their passage through matter. It involves complicated micro-interactions between an incident particle with the nuclei and electrons of the substance along their paths. Accurate stopping power data are essential for ion-beam material analysis techniques and radiation therapy (Bird & Williams, 1989; Paul, 2012). For example, in the application of quantitative analytical techniques like Rutherford Backscattering Spectroscopy and Elastic Recoil Detection Analysis, it is the stopping power that determines the depth scale in analysis and hence resolves the accuracy of analysis results. Another area with increasingly

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http://dx.doi.org/10.1016/j.eswa.2015.09.033
0957-4174/

growing uses of accurate stopping power data is radiological diagnosis and treatment. Like using standard photon beams (X-rays and gamma rays) in the ordinary radiological treatment, energetic heavy ion beam has been applied for cancer treatments in recent years (Krämer et al., 2000; Schulz-Ertner & Tsujii, 2007). When patients are irradiated with ion beams, energy is deposited into their body. The procedure is called the dose delivery. Stopping power data play a critical role in the accurate dose delivery that efficiently controls the treatment effect. The committee of International Commission on Radiological Units and Measurements (ICRU) has constantly updated a series of stopping power tabulations from protons, alpha particles and various heavy ions (ICRU, 1993; ICRU, 2005).

Despite much detailed experimental work and theoretical computations, it is still impossible to provide high precision stopping power data for every elemental projectile/target combination in the interested energy range since the number of such a combination is as many as up to a few thousands. It is also a common scenario that when a researcher needs to use a set of stopping power data related to a given projectile passing through a certain matter for an application such as ion beam analysis or materials modification, the required data may not exist. It has been highly anticipated that more data tabulations by accurate fitting are made available for a variety of projectile and target combinations. In past decades, many works have been carried out to build reliable empirical models for heavy ion stopping power data. These models were mainly based on classical nonlinear least-square algorithms incorporated quantum theory (Konac, Klatt, & Kalbitzer, 1998; Paul & Schinner, 2001, 2003; Weijers, Duck, & O'Connor, 2004; Ziegler, Biersack, & Littmark, 1985; Ziegler, Biersack, & Ziegler, 2008). Overall these studies have led up to discoveries of a number of parameterized empirical formulae that are able to predict stopping power data with varying level of agreement to experimental data.

Mathematically, curve fitting and interpolation is one class problem of two major class function approximation problems, where the unknown function is approximated by a specific class function (such as polynomial, exponential, and rational) or a set of basis functions (for example radial basis functions), given a set of data points. Interpolations based on Radial Basis Functions (RBF) have been studied for a long time. Hardy (1971) innovatively applied the multi-quadratics function to deal with surface fitting on geographical data and subsequently proved the multi-quadratics related to a consistent solution of the biharmonic potential problems. Franke (1982) surveyed various numerical algorithms on the typical benchmark data interpolation problems and concluded that the multi-quadratics RBF and thin-plate spline RBF have the superior performance in terms of efficiency and accuracy. Kansa (1990, 2000) proposed the idea of using RBF collocation scheme for solving partial differential equations and pioneered a class of meshless technique. More recently, Schaback and Wendland (2000) introduced an adaptive technique using compactly supported RBFs for solving the large scale sparse linear system problems. In past decades, RBF-based interpolations have been successfully used to solve numerous practical problems in science and engineering (Chen, Hon, & Schaback, 2007; Larsson & Fornberg, 2003; Cordero-Gracia, Gómez, & Valero, 2014; Shankar & Olson 2015; Wendland, 2010).

However, the above mentioned RBF interpolation method is not directly applicable for curve fitting problems as this method deals with the interpolating function passing through all data points and it may produce an anomalous interpolation surface due to the overdetermined problem, in which the number of data points is much larger than the number of degrees of freedom of the underlying physical system. In addition, for a noisy dataset, the exact solution of the interpolation problem often leads to an oscillating function that may give a misleading result. To overcome these difficulties, Broomhead and Lowe (1988) proposed to reformulate the RBF method by removing the restriction of exact interpolation and setting up a two-layer network architecture, where each radial basis function is served as a computation unit in the hidden layer. In this adaptive model, the training phase of network learning process is treated as the optimization of a fitting procedure for a desired surface, while the generalization of network is considered as the interpolation process of test data. Following the reformulation in the adaptive network model, RBF method rapidly gained renewed interests in computational intelligence. With a series of subsequent investigations, it has been proved that RBF networks have capability to approximate any continuous function to any degree of accuracy (Park & Sandberg, 1991; Poggio & Girosi, 1990). A class of RBF network can achieve universal approximation if the RBF is continuous and integratable (Park & Sandberg, 1991). Poggio and Girosi (1990) have reported that RBF networks possess the property of the best approximation which is not shared by multilayer perceptrons networks. Due to its superior capability of function approximation and a simple architecture, the RBF neural network has been successfully applied in many fields. The representative applications include system identification (Chen, Billings, & Grant, 1992), face recognition (Yang & Paindavoine, 2003), predictions (Han, Chen, & Qiao, 2011; Yilmaz & Kaynar, 2011), antenna design (Chen, Wolfgang, Harris, & Hanzo, 2008), and computer vision and graphics (Cho & Chow, 2001; Tsai & Shih, 2006). The performance of RBF neural network has been impressive in these applications. For example, Howell and Buxton (1998) compared RBF networks with other neural network approaches on face recognition experiments involving low-resolution video data and found that the RBF neural network had only 5–9% errors. More recently advances in RBF neural network theory and applications have been mainly focused on the improvement of algorithm efficiency and development of hybrid algorithms for various task-dependent applications (Chen et al., 2008; Constantinopoulos & Likas, 2006; Han et al., 2011; Huang, Saratchandran, & Sundararajan, 2005; Yoo, Oh, & Pedrycz, 2015; Yu, Reiner, Xie, Bartczak, & Wilamowski, 2014). For example, Yu et al. (2014) presented an offline algorithm for incrementally constructing and training RBF networks by considering an error correction procedure in each iteration. The proposed approach was evaluated on several benchmark datasets. The results showed the robustness of the method and significantly reduced the training time. It outperformed other commonly used algorithms for training the RBF networks. Yoo et al. (2015) proposed a hybrid method of incorporating the Principal Component Analysis (PCA) algorithm and RBF networks and applied to a face recognition task. In their studies, the PCA algorithm was considered to reduce dimensionality of face images while an optimized RBF network was used to identify the related pattern linked to each person. The proposed hybrid scheme obtained some unique characteristics with a better recognition rate.

Although RBF neural networks are powerful tools, one of their limitations in practice for solving a specific problem may become evident. To guarantee its best approximation property, the number of basis function should be chosen as sufficiently large. This is normally not desirable in curve fitting problems because the ultimate aim of curve fitting usually is to find a simple empirical equation with as few as possible number of parameters. If a limited number of nodes in the network is considered, the boundary behavior of the function may be deteriorated due to the localized effect from the superposition of limited number of Gaussian functions. To address this existing challenge, an extra linear neuron is introduced in the RBF network architecture. The main idea is to construct an approximation for a function by superposition of Gaussian basis functions with a linear term correction. This will efficiently balance the requirement of number of basis function and the fitting accuracy, which is one of the main contributions of this study.

The proposed RBF neural network with an additional linear neuron is investigated for fitting stopping power curves. The stopping power is the mean energy loss per unit of path length when the