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Predicting Charpy Impact Energy for Heat-Treated Steel using a Quantum-Membership-Function-based Fuzzy Model

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Abstract: This study employs quantum membership functions in a neuro-fuzzy modelling structure to model a complex data set derived from the Charpy impact test of heat treated steel for predicting Charpy energy. This is a challenging modelling problem because although the test is governed by a specific standard, several sources of disturbance give rise to uncertainty in the data. The data are also multidimensional, sparsely distributed and the relation between the variables and the output is highly nonlinear. Results are encouraging, with further investigation necessary to better understand quantum membership functions and the effect that quantum intervals have when modelling highly uncertain data.

Keywords: Heat-Treated Steel; Charpy Impact Test; Fuzzy Modelling; Quantum Membership Functions.

1. INTRODUCTION

The often large amounts of data collected from real world scenarios, combined with adequate storage space and computer processing power, have encouraged the application of data driven modelling techniques in an attempt to extract knowledge from the available information.

Information is often characterised by uncertainty which, among other considerations, is the result of parameter variations, sensor noise and measurement scatter. Often, the process to be modelled is complex giving rise to high nonlinearities, non-measurable variables and sparse data.

Modelling uncertainty is challenging, particularly with real data sets which are usually high dimensional, noisy and sometimes incomplete. Better handling of uncertainty not only improves performance and generalisation ability but, depending on the utilised techniques, may also yield models which are more interpretable leading to a better understanding of the underlying process from which the data would have been extracted. This provides better data models to the interested parties which can result in more confident decisions, better efficiency and better product quality.

In this research, we are analysing the use of quantum membership functions (Lin et al., 2004) in a new modelling framework as a way to deal with uncertainty present in data from an industrial environment.

Quantum membership functions have been employed in modelling problems, obtaining good classification accuracies (Lin et al., 2004; Lin et al., 2007). The quantum function was also considered as the activation function in neural networks (Purushothaman and Karayiannis, 1997; Kretzschmar et al., 2000). These studies indicate that quantum neural networks are able to model uncertainty by capturing the inherent structure of the data.

The data relate to the Charpy impact test and various techniques have been applied for modelling the data set being used. Tenner (1999) employed an ensemble model made up of 10 neural networks. Mahfouf et al. (2009) built a Bayesian neural network while Granular Computing is used in Panoutsos and Mahfouf (2010) where granules form a basis for Gaussian membership functions in a neuro-fuzzy structure. Yang et al. (2011) used a genetic algorithm to optimise a neural network structure with parameters from the final population providing an ensemble model.

The rest of the paper has the following outline. Section 2 introduces the data being modelled. Section 3 presents the components of the proposed modelling technique whose results are presented and analysed in Section 4. Section 5 concludes with some remarks and suggestions for future work.

2. TEST DATA

2.1 Charpy Impact Test

The Charpy impact test is a standard test used to measure the impact energy (also referred to as notch toughness) absorbed by a material during fracture. The notch provides a point of stress concentration within the specimen and improves the reproducibility of the results. The absorbed energy is computed by working out the potential energy lost by a pendulum through breaking a specimen. Results from tests performed at different temperatures are used to determine the ductile-to-brittle transition temperature of materials.

Although the test is governed by a standard test procedure, several variables influence the test result repeatability (Callister and Rethwisch, 2014; Meyers and Chawla, 2008). In fact, through convention, the test is performed on three specimens at the same temperature and the results are averaged. However, the test is still susceptible to a number of uncertainties as outlined in Lont (2000) and Splett et al. (2008), giving rise to erratically distributed data. The sources of disturbance can be grouped as follows:

- Specimen (e.g. notch geometry, inhomogeneous distribution of atoms during the early stages of nucleation, duplex grain structures including both coarse and fine grains lead to inconsistent energy distribution, chemical composition).
- System (e.g. machine stiffness and friction, calibration settings).
- Environment (e.g. ambient and specimen temperatures).
- Procedure (e.g. human error).

When combined with a highly sparse data distribution, this suggests that modelling Charpy impact test data is a challenging task.

2.2 Dataset

The heat-treated steel Charpy impact dataset used in this research was provided by Tata Steel Europe. After collecting the data, it was cleaned and pre-processed, with a metallurgist providing expert knowledge throughout this process (Tenner, 1999). The resulting data set contains 1661 samples with each record consisting of 16 input variables and the Charpy energy as output. The input variables can be grouped in three categories, which are chemical composition, heat treatment conditions and test parameters as shown in Table 1.

3. MODELLING

3.1 Quantum Membership Function

The proposed quantum neuro-fuzzy inference system uses quantum membership functions. These are characterised by the sum of a number of sigmoid functions, depending on the number of quantum levels. The sigmoid functions are shifted along the universe of discourse by the quantum intervals, resulting in multileveled membership functions. A quantum membership function is defined as (Lin et al., 2004):

$$\mu_A(x) = \frac{1}{n_\theta}\sum_{r=1}^{n_\theta}\left[\left(\frac{1}{1+\mathrm{e}^{(-\beta(x-c+|\theta^r|))}}\right)U(x;-\infty,c) + \left(\frac{\mathrm{e}^{(-\beta(x-c-|\theta^r|))}}{1+\mathrm{e}^{(-\beta(x-c-|\theta^r|))}}\right)U(x;c,\infty)\right] \quad (1)$$

where x is the input, $\mu_A(x)$ is the membership degree of x for fuzzy set A, β is the slope factor, θ^r is the quantum interval, c is the membership function centre, n_θ is the number of quantum levels and $U(x;a,b) = \begin{cases} 1 & \text{if } a \le x < b \\ 0 & \text{otherwise} \end{cases}$.

Fig. 1 illustrates the membership degree given by a three-level ($n_\theta = 3$) quantum membership function with $c = 0$, $\beta = 2$, and $\theta^r = [30,20,10]$.

The advantages of employing the quantum membership function in highly uncertain modelling scenarios are:

- A quantum set offers better generalisation through a different definition of subjectivity which would normally require multiple sets.
- A quantum membership function captures and quantifies the structure of the input space.
- The underlying data distribution can be represented by 'packets' (quanta) of similar points by the same membership degree for the particular quantum interval (level).
- The nature of the membership function having layers with the same membership degree helps to deal with outlying data points more effectively.
- Uncertainty in the data is detected and modelled by the quantum intervals which also offer another degree of freedom that can be optimised along with the other parameters.

3.2 Modelling Architecture

The modelling structure is based on the ANFIS (Adaptive Network-based Fuzzy Inference System) architecture and as shown in Fig. 2, it is similar to the type-3 ANFIS (Jang, 1993) with a TSK (Takagi-Sugeno-Kang) method of fuzzy rule inference.

Chemical Composition	**Heat Treatment Conditions**	**Test Parameters**
Carbon Silicon Manganese Sulphur Chromium Molybdenum Nickel Aluminium Vanadium	Hardening Temperature Cooling Medium Tempering Temperature	Test Depth Specimen Size Test Site Test Temperature

Table 1 - Test Variables

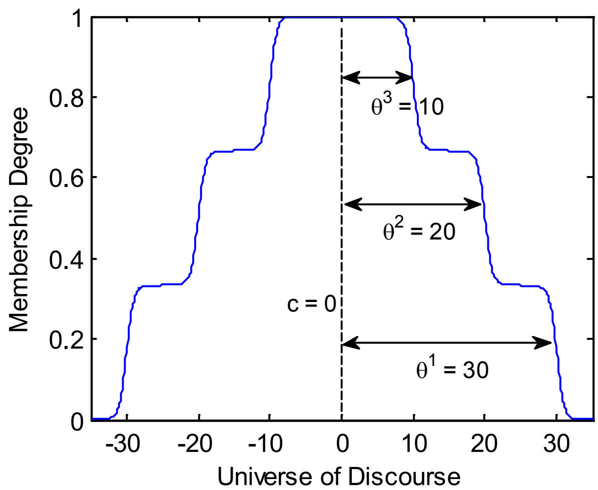

Fig. 1 - 3-Level Quantum membership function

The fuzzy if-then rules are of the form:

$$R_j: \text{ IF } x_1 \textit{ is } A_{1j} \text{ and } x_2 \textit{ is } A_{2j} \text{ ... and } x_n \textit{ is } A_{nj} \quad \text{THEN } y \textit{ is } b_j + \textstyle\sum_{i=1}^{n} a_{ij} x_i \tag{2}$$

where x_i is the input variable, y is the output, A_{ij} is the linguistic quantum fuzzy set of the antecedent part with membership degree $\mu_{A_{ij}}$, b_j and a_{ij} are the consequent parameters, n is the input dimensionality, and R_j is the j^{th} fuzzy rule.

Let q represent the number of fuzzy rules and O^l denote the output of a node in the l^{th} layer. The operations performed in each of the layers are:

Layer 1 (Membership) – The membership degree of quantum membership sets defining the linguistic variables. The number of linguistic variables for every input dimension is equal to the number of fuzzy rules which is also equal to the number of clusters. The output of this layer is:

$$O_{ij}^1 = \mu_{A_{ij}}(x_i) \tag{3}$$

Layer 2 (Intersection) – Expresses the 'AND' between premises (antecedents) which is performed through a multiplication. A firing strength for each rule is produced. An output from this layer is given by:

$$O_j^2 = \prod_i O_{ij}^1 \tag{4}$$

Layer 3 (Normalisation) – The ratio of the j^{th} rule firing strength to the sum of all rules' firing strengths:

$$O_j^3 = \frac{O_j^2}{O_1^2 + O_2^2 + \cdots + O_q^2} \tag{5}$$

Layer 4 (Consequent) – The Sugeno processing rule:

$$O_j^4 = O_j^3 \left(b_j + \sum_{i=1}^{n} a_{ij} x_i \right) \tag{6}$$

Layer 5 (Output) – Rule aggregation which is performed by summing the output from all rules:

$$O^5 = \sum_{j=1}^{q} O_j^4 \tag{7}$$

3.3 Clustering and Parameter Optimisation

Fuzzy C-means clustering was used to provide an initial estimate for the centres of the quantum sets, with the number of clusters also indicating the number of fuzzy rules.

The parameters are updated by tuning the cost function along the negative gradient to achieve supervised learning based on the error back-propagation algorithm. This is used to update the consequent parameters, b_j and a_{ij}, the membership function centres, c_{ij}, and the quantum intervals, θ_{ij}^r.

Let the cost function (for the case of a single output) be defined as:

$$E = \frac{1}{2} e^T \cdot e \tag{8}$$

where $e = y - y_t$, y is the predicted output and y_t is the target output value.

The error term to be back-propagated is described by:

$$\delta_e = -\frac{\partial E}{\partial y_t} = y_t - y = -e \tag{9}$$

The consequent parameter updates are:

$$\Delta b_j = -\frac{\partial E}{\partial b_j} = \frac{\delta_e {O_j}^3}{\sum_{j=1}^{q} {O_j}^3} \qquad \Delta a_{ij} = -\frac{\partial E}{\partial a_{ij}} = \frac{\delta_e {O_j}^3 x_i}{\sum_{j=1}^{q} {O_j}^3} \tag{10}$$

The consequent parameters are updated using:

$$b_j(k+1) = \mathrm{b}_j(k) + \eta_w \Delta \mathrm{b}_j \qquad a_{ij}(k+1) = a_{ij}(k) + \eta_w \Delta a_{ij} \tag{11}$$

where η_w is the network weight parameter learning rate and k is the time step.

Details of the centre and quantum interval updates, where the output error is back-propagated to the membership function layer, can be found in Lin et al. (2007). These result in the membership function centres and quantum intervals being updated as follows:

$$c_{ij}(k+1) = c_{ij}(k) + \eta_c \Delta c_{ij} \qquad \theta_{ij}^r(k+1) = \theta_{ij}^r(k) + \eta_\theta \Delta \theta_{ij}^r \tag{12}$$

where η_c, Δc_{ij} and η_θ, $\Delta\theta_{ij}^r$ are learning rate and update for the centres and quantum intervals respectively, and k is the time step.

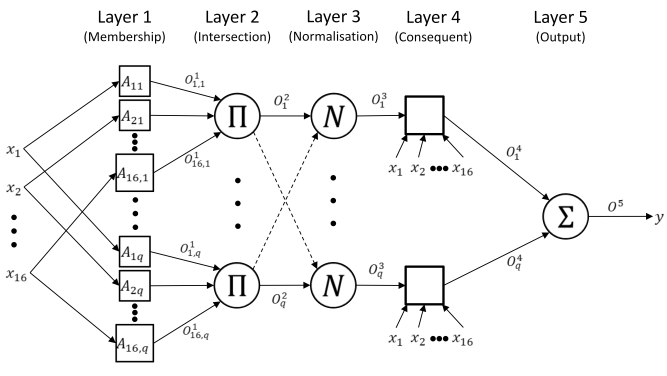

Fig. 2 - Model Structure

4. RESULTS AND DISCUSSION

The data were partitioned into training, validation and testing sets using the ratios 0.55 : 0.15 : 0.30 respectively. The data sets were then standardised using the mean and standard deviation of the training data.

Clustering was performed on the dimensions separately. This is because when clustering across all variables, the centres were random across the range of each variable. However, clustering the variables individually resulted in more specific points being chosen as centres.

The number of clusters, which corresponds to the number of rules in the model, was varied between 3 and 10. Several models for the quantum-based architecture were tested for each cluster setting and the results were averaged to allow comparison between the different architectures. Considering both the performance and the times when the model optimisation diverged, it was decided to use a model with 6 rules. Table 2 presents the results for a model with 6 clusters, with a resulting correlation coefficient of 82% between the real and predicted outputs for the testing data as shown in Fig. 3. The low variation in RMSE across the three data sets indicates that the model performs consistently on the data.

These results are comparable with those obtained in previous publications using the same dataset (Tenner, 1999; Mahfouf et al., 2009; Panoutsos and Mahfouf, 2010; Yang et al., 2011) which are summarised in Table 3.

5. CONCLUSION

In this paper, promising modelling results were obtained using a Quantum-membership-function-based fuzzy model to predict Charpy energy for data obtained from the Charpy Impact test.

Fig. 4 shows a plot of the membership functions across the data variables. Although the number of quantum levels was fixed to 3 per membership function, it can be noticed that few of them exhibit evident quantum levels. This indicates that while the model was able to capture the uncertainty in the data, more research is required to understand the effects of quantum levels in these membership functions. This can be done by restricting the membership function widths and fixing some of the levels. Further changes that can be made to the model stem from whether it has a smooth or coarse decision surface with respect to the input variables. This is influenced by the shape of the membership functions and has an effect on the performance of the model.

Different optimisation procedures can also be implemented such as optimising and then fixing the parameters of the different sections of the model separately, and using an adaptive optimisation algorithm. To better understand the membership functions, a simpler model may also be used such as one based on a Mamdani-type fuzzy logic structure.

	Training data	**Validation data**	**Testing data**
Correlation Coefficient	0.835	0.787	0.822
RMSE (Joules)	17.75	18.84	18.17

Table 2 - Model Performance

	RMSE Training Data	**RMSE Validation Data**	**RMSE Testing Data**
Ensemble NN (i)	13.2	17.1	18.3
BNN (ii)	17.31	20.77	19.49
GrC-NF (iii)	14.66	21.24	20.42
GA-NN Ensemble (iv)	13.12	17.25	18.13

(i) Tenner, 1999; (ii) Mahfouf et al., 2009; (iii) Panoutsos and Mahfouf, 2010; (iv) Yang et al., 2011

Table 3 - Past results of Charpy impact energy prediction

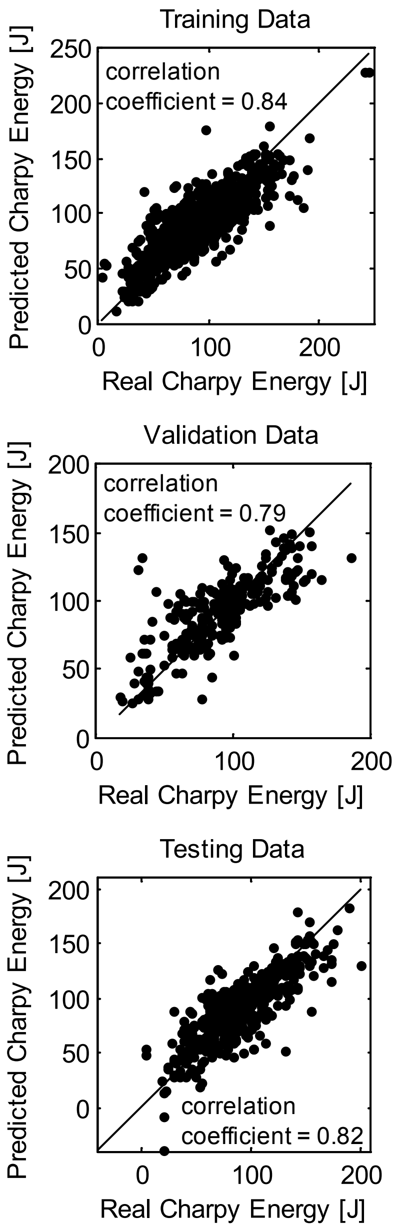

Fig. 3 - Charpy Energy Prediction

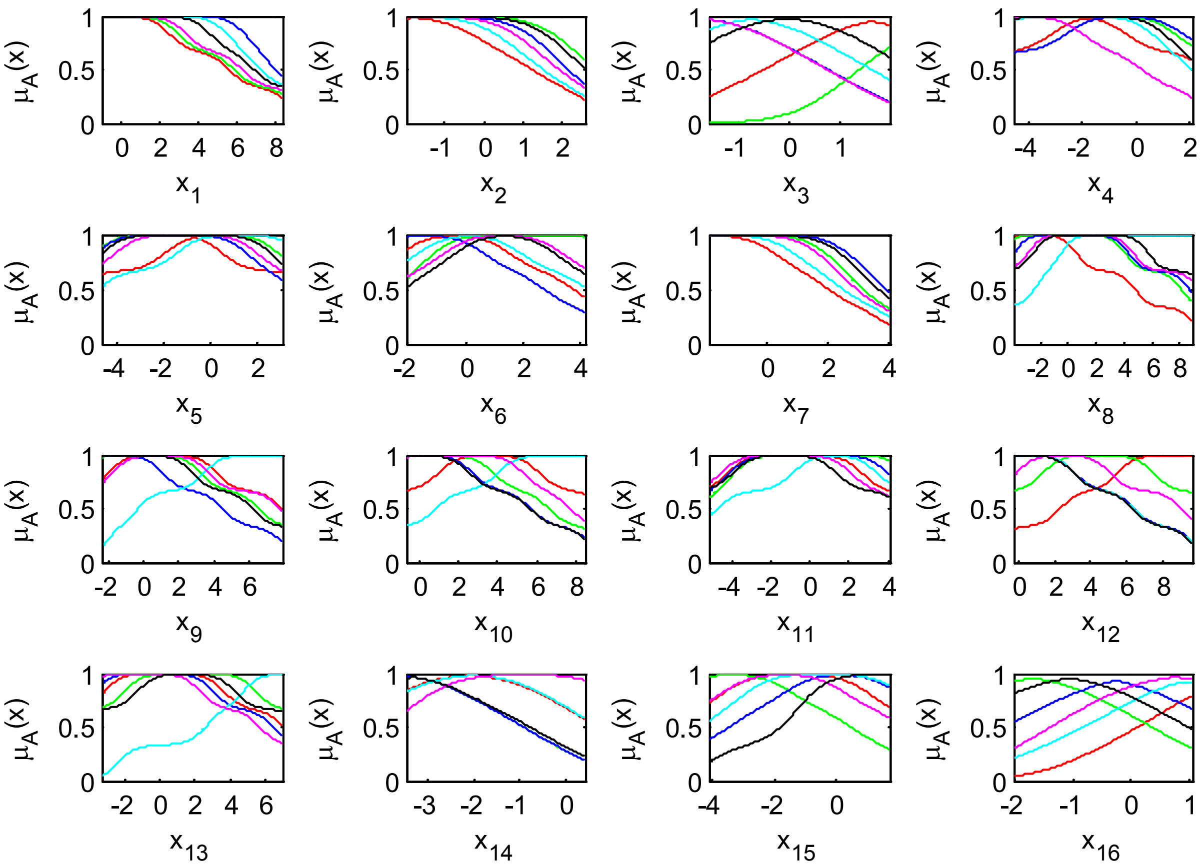

Fig. 4 - Membership Functions for the Charpy impact data input variables

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