Data Mining and Modelling of Charpy Impact Energy for Alloy Steels Using Fuzzy Rough Sets

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Abstract: When considering data-driven modelling, uncertainties, errors and inconsistencies in the data can more often than not lead to sub-optimal predictions. A new framework based on rough sets theory is proposed and applied to an industrial data set obtained from a Charpy impact energy test for alloy steels. The inconsistent/consistent data sets are then used to train a series of artificial neural networks (ANN) for Charpy impact energy prediction for alloy steels. A k-nearest neighbor is used to classify the data points; if an object is classified as consistent, the ANN trained with the consistent data set provides a single prediction while if the object is classified as inconsistent, several ANN trained with different sets of inconsistent data are used to provide an interval prediction. Experimental results show an improvement in the consistent data set compared with a benchmark model. Also, the interval prediction provided by the various ANNs in the inconsistent data set represents a better alternative to the single point prediction results.

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Keywords: Charpy impact energy, neural networks, classification, fuzzy sets, rough sets, data-driven model

1. INTRODUCTION

The demand for better materials with specific properties and the current situation in the global market makes it necessary to reduce cost in steel production by achieving a right-first-time production. Material properties prediction is a challenging task, due to the complex interactions between material process, structure and properties. First principle formulations usually are not capable of capturing these interactions therefore data driven-models have become a common solution for material prediction, due to the availability of large data sets obtained from materials testing. These data sets, similarly to most information obtained from real systems, is usually corrupted by noise and other errors making it increasingly necessary to apply concepts of data mining and machine learning to aid the modelling process.

Previous research has been conducted in modelling Charpy impact energy including neuro-fuzzy models (Chen and Linkens, 2006), granular computing (Panoutsos and Mahfouf, 2010), Gaussian mixture models (Yang et al., 2011a). Research in rough set theory applied to materials science is scarce and its potential to model vagueness and uncertainty in a system has not yet been fully studied.

The Charpy impact test is used in the industry due to its capacity to obtain large amount of data in a relatively short space of time and its low costs. It is used to characterize the ductile-to-brittle transition of a material by measuring the energy absorbed by the material during fracture at different temperatures. Samples evaluated in a Charpy impact test are impacted by a pendulum, and the difference between the potential energies before and after the impact is associated to the energy absorbed during fracture (Meyers and Chawla, 2009).

The ductile-to-brittle transition occurs at different temperatures; lower temperatures are associated with a low impact energy and brittle fracture, while high temperatures are associated with high impact energy and ductile fracture.

The samples are obtained from different sections of the specimen being studied, and must be placed in the test machine at a determined temperature. Due to the material microstructure anisotropy and the ductile-to-brittle transition the data obtained usually include significant inconsistencies.

Objects in a data set are considered inconsistent when the attribute values of two or more objects are the same or similar and the output differs. Inconsistencies in a data set are the product of error in measurements or variables that are not being taken into consideration (lack of knowledge). Rough set theory is used in this work to identify and quantify inconsistent objects in the data set.

Rough set theory was specifically developed to model vagueness and uncertainty in data. Classical rough set theory works only with qualitative data, leading to limitations when dealing with quantitative data sets. Because of these limitations researchers have developed fuzzy-rough sets. Rough set theory and fuzzy rough set theory have been implemented in pattern recognition, attribute reduction, rule induction, classification, knowledge discovery (Qamar, 2013, Jackson et al., 1998, Jensen and Shen, 2009, Jensen and Shen, 2007, Bag et al., 2014, Huang, 2010). The aim of this research is to propose a new data-mining framework that is capable of: 1. identifying inconsistencies in data sets; 2.

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10.1016/j.ifacol.2017.08.2555
classifying objects pertaining to a consistent or inconsistent region; 3. providing a set of approximate results to elicit a prediction interval instead of a single point prediction in regions identified previously as inconsistent in order to quantify uncertainty in the system and improve prediction accuracy.

The remainder of this paper is organized as follows: Section 2 contains a brief overview of Rough set and fuzzy rough set theory, k nearest neighbour classification algorithm and artificial neural networks. Section 3 describes the data set and the inconsistencies included within. Section 4 describes the framework created in this research while Section 5 the results obtained with discussions. Finally, section 6 draws the necessary conclusions.

2. BACKGROUND

2.1 Rough Set Theory

Rough set theory was established by Pawlak (Pawlak, 1982). Rough sets are used to model uncertainty and vagueness in an information system. Rough sets consist of two approximations; an approximation which includes objects that belong to a set \( X \) called the lower approximation and an approximation that includes objects that might belong to a set \( X \) called the upper approximation. These approximations are created based on the indiscernibility relationship between objects in a decision system, that is, due to lack of knowledge in an information system it is not possible to discern between two or more objects and therefore are treated in the form of information granules.

In an information system \( I = (U, C, V) \) where \( U \) is the universe of discourse, \( C \) is a set of conditional attributes and \( V_c \) is a set of values the attributes might take. Given any subset \( P \) of \( C \) conditional attributes the indiscernibility relation between objects is as follows:

\[
\text{IND}(P) = \{ (x, y) \in U^2 \mid \forall c \in P, c(x) = c(y) \} \tag{2.1}
\]

Objects that are indiscernible are represented in a P-elementary set \( [x]_P \). Given any subset \( X \) of the universe of discourse \( U \) the lower and upper approximation are respectively:

\[
\underline{PX} = \{ x \mid [x]_P \subseteq X \} \tag{2.2}
\]

\[
\bar{PX} = \{ x \mid [x]_P \cap X \neq \emptyset \} \tag{2.3}
\]

The tuple \( (\underline{PX}, \bar{PX}) \) is defined as the Rough set. Figure 1 provides a graphical representation of a Rough Set.

![Rough set representation](image)

2.2 Fuzzy Rough Set Theory

Since the early development of the classical rough set theory several attempts have been made to develop fuzzy-tough sets hybrids. The classical rough sets only deal with qualitative data. Most real valued data sets contain quantitative data which may lead to serious limitations for their exploitation. The first successful attempt at fuzzy rough sets were developed by Dubois and Prade, (1992), where they developed fuzzy partitions in the data set itself. The main problem with their method relates to the computation costs, therefore it will not be used in this work. The scheme used in this work was introduced by Radzikowska and Kerre, (2002). Instead of measuring the indiscernibility relationship between objects a measure of their similarity is instead calculated using a fuzzy tolerance relationship \( \mu_{R_c} \). The fuzzy-rough lower and upper approximations are as follows:

\[
\mu_{R_c}^{\underline{L}}(x) = \inf_{y \in U} (\mu_{R_c}(x, y), \mu_{c}(y)) \tag{2.4}
\]

\[
\mu_{R_c}^{\bar{L}}(x) = \sup_{y \in U} (\mu_{R_c}(x, y), \mu_{c}(y)) \tag{2.5}
\]

\[
\mu_{R_c}(x, y) = \bigcap_{c \in P} [\mu_{c}(x, y)] \tag{2.6}
\]

Where \( T \) is a t-norm, and \( I \) is a fuzzy implicator. \( \mu_{R_c} \) is a similarity measure between objects \( x \) and \( y \) for a feature \( c \). In this work the, the Łukasiewicz t-norm (2.7), the Łukasiewicz implicator (2.8) and the fuzzy similarity relations (2.9) are used (Jensen and Shen, 2009).

\[
T = \max(x + y - 1, 0) \tag{2.7}
\]

\[
I = \min(1 - x + y, 1) \tag{2.8}
\]

\[
\mu_{R_c}(x, y) = \exp \left( \frac{(c(x) - c(y))^2}{2\sigma_c^2} \right) \tag{2.9}
\]

Where \( \sigma_c^2 \) is the variance of attribute \( c \).
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