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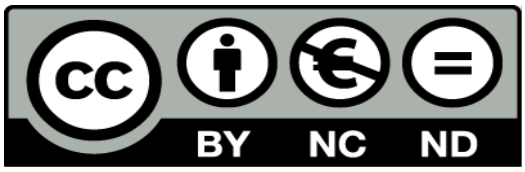

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Development and Application of Soft Computing and Data Mining Techniques in Hot Dip Galvanising

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I hereby declare that this thesis entitled "Development and application of Soft Computing and Data Mining techniques in Hot Dip Galvanising" is the result of my own research except as cited in the references. This thesis has not been accepted for any degree and is not concurrently submitted in candidature of any other degree.

Signature :

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Date : December 2012

Supervisor : Dr. Francisco Javier Martínez de Pisón Ascacibar

For my beloved mother

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I would like to start these acknowledgements saying 'thank you' to my mother Carmen for her love and the possibilities she has created for me, and my brother Iñigo who has always helped me. I would also like to thank those who over the years have given me their friendship but they are too numerous to mention all of them here. Other members of my family, many friends and particularly Almudena, whose constant encouragement and great patience have been there through all the difficult times.

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Andrés Sanz García, Logroño

Abstract

In a world in which markets are more globalised and continuously evolving, companies need new tools to help them enhance their flexibility to maintain their competitiveness. To this end, a key strategy is the discovery of useful knowledge through the information gathered from businesses and production processes. In recent decades, many companies that are aware of this necessity have increased their investments for improving both data storage capacity and information management. Currently, the huge volume of information stored by companies and its high complexity render traditional methods of data processing useless, posing serious problems for industry. However, the use of accurate tools to extract the information hidden inside industrial databases, and then transform it into explicit knowledge, is still under development. The creation and application of such methodologies will make the key points of industrial processes more flexible, and thereby fulfil the needs of global markets.

With the aim of solving this problem, new computer-based methodologies derived from data mining are being developed. By using these methods, researchers are seeking to obtain non-trivial hidden knowledge from historical records of industrial processes. For this reason, data mining has now become a crucial discipline for performing automatic searches inside historical industrial databases, contributing to industrial development and advancement. Data mining involves several techniques from different disciplines, such as statistics, machine learning and artificial intelligence, among others.

This thesis focuses on the use of data mining techniques to develop helpful semiautomatic methods for tuning industrial production lines. The goal is to increase flexibility in industrial processes in response to the need to meet new consumer expectations and continue being competitive. The methodologies developed have been used to study and improve a continuous galvanising line.

Bearing in mind its complexity, our aim is to explore the opportunities that data mining techniques can offer for improving this industrial process.

The techniques used during the writing of this thesis are classified into two categories: descriptive, for association rule mining; and predictive, for modelling based on soft computing. Soft computing is defined as "obtaining solutions by the use of intelligence, common sense or approximation by emulating human behaviour".

The goal of the first part of this thesis is to seek novel non-trivial knowledge in the form of patterns to help explain failures in production lines. To this end, an overall methodology that integrates both data management and association rule mining is proposed. Our aim is to capture those frequent events that coincide when there is a failure in the industrial process studied.

The second part focuses on improving the modelling of non-linear dynamic systems using historical information from industrial processes. In this case, the strategy is based on combining different soft computing techniques. The techniques developed are designed to improve the estimation of temperature set points for an annealing furnace on the galvanising line studied.

The contributions presented in this doctoral thesis provide evidence of the huge potential that data mining has for obtaining useful, comprehensible knowledge from industrial processes.

Resumen

En un mundo donde los mercados son cada día más globales y cambiantes, la industria necesita del apoyo de nuevas herramientas para mejorar su flexibilidad operacional y continuar manteniendo altos niveles de competitividad. Una estrategia clave para esta mejora es la búsqueda de conocimiento útil a partir de la información procedente de sus procesos productivos y empresariales. En las últimas décadas, las empresas han realizado importantes inversiones para mejorar el almacenamiento y procesado de dicha información. Sin embargo, aún es muy incipiente en la industria, la implementación de herramientas que extraigan el conocimiento implícito subyacente en su información almacenada para transformarlo en explícito, permitiendo así flexibilizar sus procesos.

Debido al volumen de información almacenada y su elevada complejidad, los métodos tradicionales de procesamiento de datos no pueden ser empleados hoy en día. Esto representa un grave problema para la industria. Por ello, se están desarrollando metodologías basadas en el uso de computadoras para obtener conocimiento útil a partir de datos históricos de procesos industriales. La minería de datos se ha convertido en una disciplina crucial para realizar esta búsqueda de forma automática en grandes bases de datos. Esta disciplina se nutre de numerosas técnicas procedentes de otras tales como la estadística, el aprendizaje automático y la inteligencia artificial entre otras.

Con la realización de esta tesis doctoral se pretende desarrollar metodologías basadas en minería de datos que ayuden al ajuste de las líneas de producción industrial. El objetivo es conseguir mayor flexibilidad y eficiencia en la fabricación de nuevos productos. Para demostrar su aplicación práctica, las metodologías propuestas han sido empleadas en el estudio y mejora de una línea de galvanizado continuo por inmersión en caliente de bobinas de acero. La dimensión y complejidad de la misma pretenden poner de manifiesto las oportunidades que ofrece la

minería de datos en la mejora de este proceso industrial.

Las técnicas empleadas en la realización de esta tesis se engloban bajo dos categorías diferentes: descriptivas para la extracción de reglas de asociación, y predictivas, basadas en Soft Computing, con el objetivo de modelar sistemas. Soft Computing se puede definir como "la obtención de soluciones mediante el uso de la inteligencia, el sentido común o la aproximación por imitación a los seres humanos".

El objetivo de la primera parte de esta tesis doctoral ha consistido en la extracción de conocimiento útil y no trivial en forma de patrones que permitan explicar fallos frecuentes en líneas de producción. Para ello, se propone una metodología global que integra tratamiento de datos y minería de reglas de asociación para mostrar eventos que aparecen con alto grado de coocurrencia cuando se producen fallos en el proceso.

La segunda parte se ha centrado en la mejora del modelado de sistemas dinámicos no lineales a partir de datos históricos del proceso industrial. En este caso, se desarrollaron dos metodologías basadas en la combinación de distintas técnicas de Soft Computing. Estas metodologías permitieron mejorar la estimación de las temperaturas de consigna del horno de recocido de la línea de galvanizado estudiada.

Las contribuciones presentadas en esta tesis doctoral demuestran el enorme potencial de la minería de datos a la hora de proporcionar conocimiento útil y comprensible a partir de datos históricos de procesos industriales.

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List of Symbols and Nomenclature

χ	mutation factor
η	learning rate of back propagation alg.
μ	weighting coef. of complexity term
Al, Cu, Ni, Cr, Nb	chemical composition of steel (in percentage of weight)
C, Mn, Si, S, P	chemical composition of steel (in percentage of weight)
$Conseq$	consequent
CV	coefficient of variation
E	event sequence dataset
G	total number of generations
H	number of neurons in hidden layer
I	num. of best indiv. for early stopping
J	fitness function
M	momentum of back propagation alg.
MAE	mean absolute error
ME	mean - superscript -
N	total num. of simulations for models
P	population size
q	binary array for feature selection

R	compression rate
R^2	Pearson´s correlation coefficient
$RelConfidenceWinRule$	relative confidence within a time window
$RelSupportWinRule$	relative support within a time window
$RMSE$	root mean squared error
SD	standard deviation - superscript -
T	transactional episode database
t	comp. cost for training models
T_g	period of stability
$THC1$	Zone 1 Set Point Temperature (ºC)
$THC3$	Zone 3 Set Point Temperature (ºC)
$THC5$	Zone 5 Set Point Temperature (ºC)
$ThickCoil$	strip thickness at the annealing furnace inlet (mm)
$TimeLag$	window time-tag (ut)
$TMPP1$	strip temperature at the heating zone inlet (ºC)
$TMPP2$	strip temperature at the heating zone outlet (ºC)
$TMPP2CNG$	strip temperature at the heating zone outlet (ºC)
V, Ti, B, N	chemical composition of steel (in percentage of weight)
$VelMed$	strip velocity inside the annealing furnace (m/min^{-1})
W	complexity term
$WidthCoil$	strip width at the annealing furnace inlet (mm)
$WinW$	window width (ut)
x_e	elitism percentage
x_g	fraction for adjusting penalty function
x_{CI}	proportion of confidence interval
x_{val}	proportion of validation data

AI	artificial intelligence
ANN	artificial neural network
AR	additive regression
ARM	association rule mining
BG	bootstrap aggregating (bagging)
CAF	continuous annealing furnace
CHDGL	continuous hot dip galvanising line
DB	database
DG	dagging
DM	data mining
EC	evolutionary computing
EM	ensemble method
ESC	early stopping criterion
FS	feature selection
GA	genetic algorithm
GA–NN	genetic algorithm guided neural network
KDD	knowledge discovery in databases
KM	knowledge management
k-NN	k-nearest neighbour
LMSQ	least median squared linear regression
LR	linear regression
MLP	multilayer perceptron

M5P	Quinlan´s improved M5 algorithm
RBFN	radial basis function network
SC	soft computing
SVM	support vector machine
PCA	principal component analysis
TDB	transactional database
TDM	temporal data mining
TS	times series
TSKR	time series knowledge representation
UT	unification-based temporal

Chapter 1

Introduction

The maximisation of profits from existing plants is a constant in steel industry due to the large investments and long-term payback times of new plants. Steel companies constantly need to cut costs while increasing productivity, with no reduction in product quality (Okereke & McDaniels, 2012; Madureira, 2012). In such a context, an organisation´s goal is to select optimal strategies to ensure the maximisation of profits in all circumstances (Hoppe, 2002; Moffat, 2009; Cheng *et al.*, 2009). However, the selection is not so easy matter and has started to become a serious problem in today´s globalised and ever-changing markets (OEC, 2006; Int, 2010).

One way of overcoming this problem is to develop new tools that help steel companies to gain deeper insights into their operations (Malerba, 2007; GmbH, 2009; Lee *et al.*, 2009). A better understanding of the "underlying principles" of their processes would allow companies to increase their intellectual capital and make them more competitive (Harvey & Lusch, 1999; Femminella *et al.*, 1999; Lee *et al.*, 2012; Lengnick-Hall & Griffith, 2011).

In recent decades, companies have started to become aware of this need to increase their intellectual capital, making large investments in data acquisition, data storage and information processing systems (Erickson & Rothberg, 2009; Lücking, 2011). As data-capture and data-storage technologies are comparatively low cost, a common characteristic of modern factories is now exponential growth in size of their databases (DBs), which contain large volumes of data from their processes (see Figure 1.1).

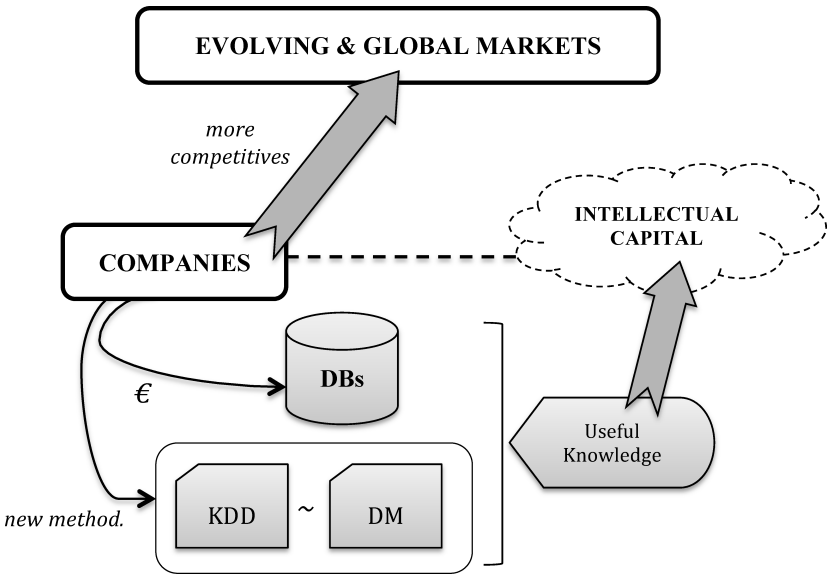

Figure 1.1: Basic scheme of actual framework of companies and DM tools

This huge amount of data theoretically contains hidden knowledge that could help companies to gain competitive advantages in current markets by explaining multiple failures in their processes (Alfonso-Cendón *et al.*, 2010), estimating product properties on-line (Ordieres *et al.*, 2004), identifying relevant features that compromise product quality (Agarwal & Shivpuri, 2012), helping to predict process set points (Jelali, 2006), and so on. Indeed, the data stored seems to contain an incredible potential that has been widely investigated by many researchers (Hodgson, 1996; Kusiak & Zuziak, 2002; Bloch & Denoeux, 2003; Li & Dong, 2011), although it is agreed that raw information is rarely of direct benefit (Harding *et al.*, 2006; Köksal *et al.*, 2011).

Companies have traditionally used manual procedures performed by process analysts to handle their DBs and prepare reports, extract conclusions, discover rules or undertake other tasks related to knowledge management (KM). There is now more evidence than ever that processing data collected from company processes using only traditional methods is wholly unfeasible because of their size. Consequently, this has led to the need to discard manual methodologies in favour of automatic tools (Schiefer *et al.*, 1999; Ordieres *et al.*, 2004).

Analysts and experts also stress that the scale of the problem will steadily an increasingly outpace human capacities. The avalanche of information will render it more difficult to extract useful conclusions underpinning today´s decision-making procedures (Kantardzic, 2011). This phenomenon has triggered corporate interest in developing new automatic computer-based methodologies that efficiently deal with large DBs to extract useful knowledge. Questions re-

garding the most suitable techniques for discovering hidden knowledge are often solved by focusing attention on existing facilities (Aldrich, 2002).

A promising approach to this problem, and one that exploits the huge quantity of historical records stored in DBs today, is the application of techniques of knowledge discovery in databases (KDD) (Maimon & Rokach, 2008). KDD is concerned with the task of extracting non-trivial useful knowledge from large volumes of data (Mannila, 1997). This multi-disciplinary field is frequently described as "mining information from the input data" and in fact, the essential step in KDD is called data mining (DM). The two fields are very closely related in terms of methodology and terminology (Mitra *et al.*, 2002).

The actual DM task is defined by Hand *et al.* (2001). DM can automatically identify interesting patterns in large volumes of data and try to extract knowledge from them, transforming the original data into an understandable structure of information for further use (Chapman *et al.*, 2000). In recent years, this field has started to be widely used in many disciplines of engineering and science, such as electrical power engineering, bioinformatics, medicine and geography.

In practise, DM involves the application of low-level algorithms to reveal hidden information in large volumes of data (Miller & Han, 2001; Han & Kamber, 2006). Nevertheless, the implementation of the DM process is definitely not an easy task, since most of the DM techniques are independent and their combination does not often lead to better solutions. As Yang & Wu (2006) indicate, the potential of these techniques is still unknown and we are far from answering such questions as wether we can discover Newton´s laws from observing the movements of objects.

There is a fair amount of evidence (Cox *et al.*, 2002; González-Marcos, 2007; Martínez-De-Pisón, 2003; Maimon & Rokach, 2008) showing that DM is a promising approach to which the steel industry is turning its attention. Many authors posit (Marakas, 1998; Giudici & Figini, 2009) that DM has unique properties that may enhance competitive advantages if developed for such industrial domains. However, although there have been several encouraging results, the real world is often far from ideal, and DM is currently an open research topic (Köksal *et al.*, 2011). Without developing efficient methodologies, the DM techniques themselves and the effort required to collect the data from a real problem do not provide commercial advantages to companies in industrial domains (He *et al.*, 2009).

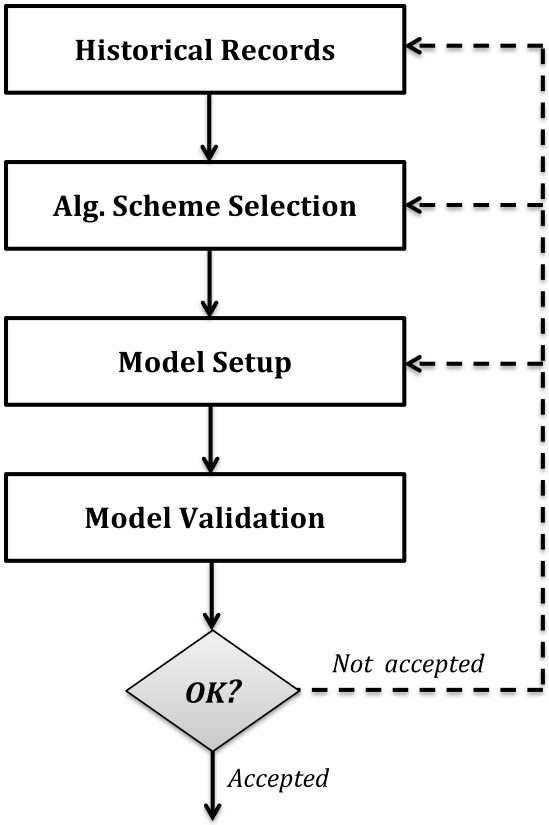

Figure 1.2: Basic procedure for developing models (from Norgaard et al., 2003)

On one hand, the massive times series (TS) captured from industrial environments are generally contaminated by noise. The conditions at industrial plants create many inaccurate and spurious data (outliers) due to electromagnetic interferences, phantom loads, power-line surges from plant machinery, etc. Handling noisy data and simultaneously gathering meaningful information from them render the DM process more complex. Although major advances have been reported in pre-processing of TS, tasks such as the automatic elimination of outliers or noise filtering are still extremely difficult (Dürr *et al.*, 2005).

On the other hand, most of industrial TS must be considered as non-static and unbalanced data that are far from being independently and identically distributed (iid). This is because historical records from processes are usually composed of many variables of different types with multiple non-linear relations.

New automatic or semi-automatic methodologies based on DM should deal with all the factors described above. With minimal human assistance, they have to solve the industrial problem for which they were created. These issues mean their development and subsequent implementation are extremely challenging. Additionally, our aim here was to obtain a reliable evaluation. We thus

extended our list of goals to include a final task of applying the methodology to a real industrial case. The evaluation consisted of a list of criteria for assessing how our methodology performed in real situation (see Figure 1.2).

In order to evaluate the proposals, a list of process candidates of proven significance within the steel industry was generated. The case study, details of which are provided below, was finally selected from this list, taking into consideration mainly its complexity, the availability of real data and the existence of plant experts. Some phenomena in industrial processes are not so readily understandable. There are several specific cases in which explanations require complex descriptive structures or non-linear predictive models. Moreover, the problem of finding the latent structure of these phenomena is very challenging due to the high-dimensional data collected.

This thesis focuses on the use of DM techniques to develop helpful semi-automatic methods for tuning industrial production lines. Our goal is to increase flexibility in industrial processes to fulfil new consumer expectations quickly in order to continue being competitive. The methodologies developed have been used to study and improve a continuous galvanising line.

A continuous hot dip galvanising line (CHDGL) is a clear example that featuring all the problems and requisites that we seek to address in this thesis (Bian *et al.*, 2006; Mullinger & Jenkins, 2008). From an economic and strategic point of view, CHDGL is a key process for steel companies. They have made important investments to increase production by automating the entire process and reducing the number of operations in which humans operators are involved. The automation process has brought new problems and the situation is now becoming more serious owing to a steady increase in the demand for cheaper rolled flat steel products.

The need to produce high quality galvanised products without decreasing line capacity has also created a need for additional improvements in the automation systems, such as more reliable on-line monitoring systems and accurate models for predicting process set points (Zhong *et al.*, 2002; Suarez *et al.*, 2010), for example.

Historically (Ueda *et al.*, 1991), improvement in the monitoring and control system in CHDGLs has been based largely on mathematical models that have usually been implemented instead of expensive plant trials (199, 1998; Tian *et al.*, 2000).

The initial motivation for this thesis is based mainly on the previous work of Bloch *et al.* (1997), Schiefer *et al.* (1999), and Martínez-De-Pisón (2003). These publications mark a change in the direction from mathematical approach, developing new models to replace previous ones. From the very outset, the results of these initial papers began to reveal more accuracy and reliability than traditional techniques (Ordieres *et al.*, 2004, 2005; Pernía-Espinoza *et al.*, 2005; Li *et al.*, 2006; Pal *et al.*, 2006; González-Marcos, 2007), generating a research field in which many improvements have been widely reported in different components of CHDGL (Martínez-De-Pisón *et al.*, 2006, 2010a).

Two recent papers (Martínez-De-Pisón *et al.*, 2010b, 2011) that improve the prediction of the temperature set points in a continuous annealing furnace (CAF) and an additional work (Ordieres-Meré *et al.*, 2010) predicting the properties of galvanised steel strip are considered as the basis for the work presented in this thesis. Furthermore, following the good performance achieved with the proposals made in those papers, there is still ample scope for improvement, especially in robustness, reliability and the capacity for generalisation in predicting novel data. This has been shown in recent research into different approaches such as evolutionary artificial neural networks (ANNs) (Yang *et al.*, 2011), support vector machines (SVMs) (Liu *et al.*, 2011) and ensemble methods (EMs) (Pardo *et al.*, 2010; Niu *et al.*, 2011; Okun, 2011)

A further aim was to provide qualitative information about the CHDGL (Choo *et al.*, 2007). We thus developed new descriptive models as another of our goals. Detecting and identifying the causes of frequent failures in CHDGLs is essential to ensuring plant productivity and the product quality of galvanised strip surface (Xu *et al.*, 2009; Li *et al.*, 2011a).

By drawung on the knowledge of plant engineers and using DM-based approaches (Alfonso *et al.*, 2012), several applications have been focused on this specific problem (Gonzalez *et al.*, 2006; Zhang *et al.*, 2010). Through this alternative approach, the research is closely related with other previous publications, such as (Alfonso-Cendón *et al.*, 2010; Posada, 2011; Ferreiro *et al.*, 2011).

1.1 Continuous hot dip galvanising and annealing furnace

CHDGL is briefly described in this section because the experimental validation of our methodologies lies in the historical records from a real galvanising line

located in northern Spain.

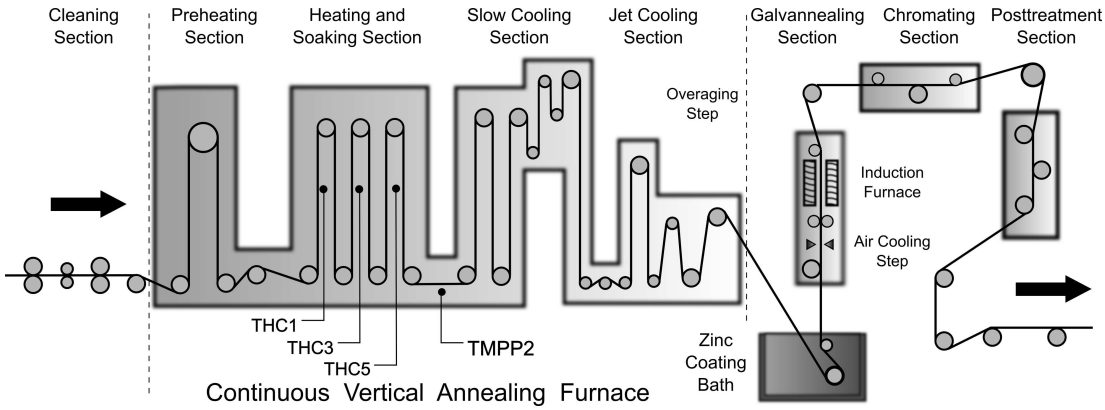

Figure 1.3: Simplified scheme of a continuous hot dip galvanising line

Galvanised steel is widely used due to its corrosion protection in many applications, such us automotive body parts, electrical transmission and appliance industry (Rentz & Schltmann, 1999). The process of galvanising steel products is broken down according to its technology into continuous and discontinuous, but continuous process is the only one used to coating steel coils and also the more economical for mass output (González-Marcos, 2007).

Broadly speaking, the different continuous galvanising lines can be classified into the following three types: combined annealing and galvanising line, hot dip galvanising line and hot strip continuous galvanising line (Ame, 2006). The second type of line involves applying a zinc coating to steel products to protect the steel from corrosion by immersing the preheated material in a bath consisting primarily of molten zinc.

This thesis focuses on a continuous hot dip galvanising process for steel coils. This technology has several advantages over others, such as relatively low costs and high volume production (Martínez-De-Pisón, 2003). However, as mentioned earlier in Chapter 1, most of the research in this thesis is directly related to the CAF on the CHDGL studied, which is the heart of the annealing process (Pernía-Espinoza *et al.*, 2005).

A CHDGL for steel coils contains mainly five separate sections that perform a particular treatment on the steel strip during the process (Figure 1.3):

1. Pre-heating area

2. Heating and holding area

3. Slow cooling area

4. Jet cooling area

5. Overaging area

The following paragraph describes the particular process that was selected as case of study in this thesis. However, the description can be applied, with certain minor modifications, to other industrial plants worldwide.

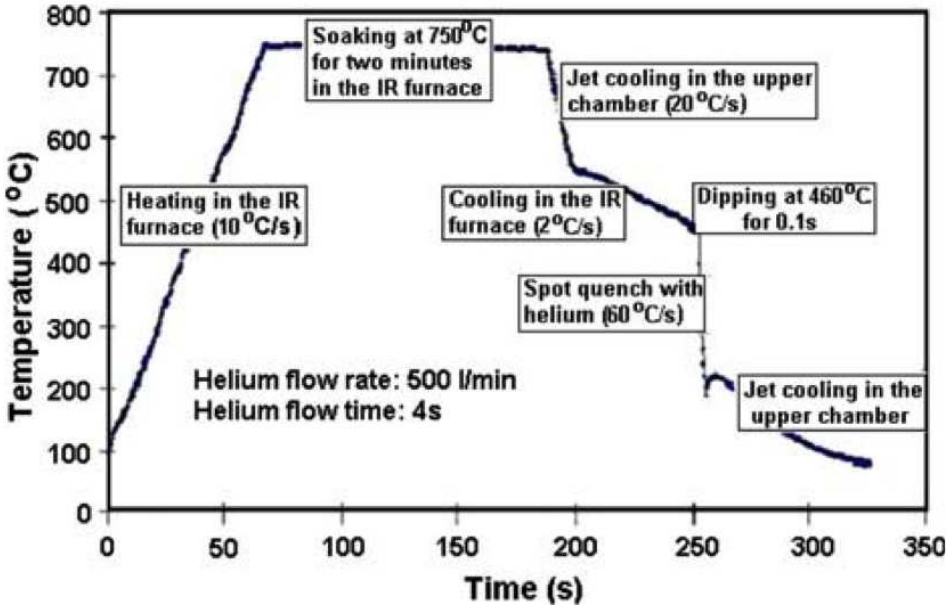

Figure 1.4: Thermal galvanising cycle in CHDGL (from Chen et al., 2008)

First, initial steel coils from the cold-rolling process need to be unwound, welded together to form a continuous strip and cleaned, then fed into the annealing furnace. Once the steel strip is inside the furnace, it runs through a number of vertical loops to obtain pre-established temperatures according to an annealing cycle. The steel strip subsequent passes through a molten zinc coating bath followed by an air stream "wipe" that controls the thickness of the zinc coating. Finally, the strip is treated by a series of auxiliary processes, forming a coil shaped product.

The initial surface preparation of the base metal is critical for maintaining the quality of the galvanised steel products. Nevertheless, three additional zones also have to be controlled to ensure the uniformity of the zinc film in an immersion process: the molten zinc bath, the CAF, and the air-cooling jet. Note that a more detailed description of the galvanising line is provided in Vergara (1999).

The annealing treatment is applied to the steel strip to heat it and main-

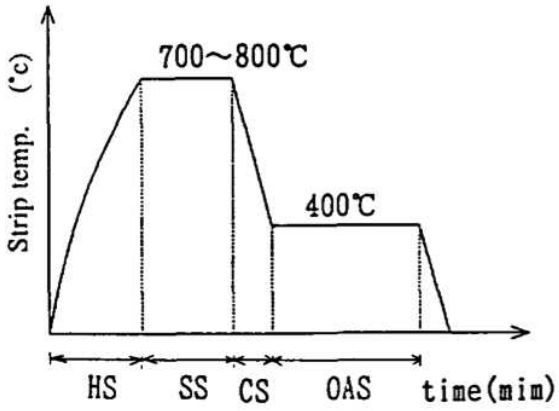

Figure 1.5: Thermal annealing cycle in a CAF (from Ueda et al.*, 1991)*

tain it at an appropriate temperature, followed by a cooling process at different rates. In short, each cold rolled coil has to be subjected to a heat treatment to improve its mechanical properties and the uniformity of the zinc coating (Tang, 1999). Figure 1.4 and Figure 1.5 show two examples of different profiles of annealing cycles, a thermal cycle for steel samples in a CHDGL (Chen *et al.*, 2008) and strip temperature cycle in a CAF (Ueda *et al.*, 1991), respectively.

The standard control of the CAF usually involves maintaining the strip velocity within a pre-established range of values while managing the temperature settings in each zone (Yoshitani & Hasegawa, 1998). Today, the efficient and cost-effective operation of a CAF is unimaginable without integrated automation systems. The introduction of improved automation systems or better furnace regime controls allows the line speed and, consequently, its ouput to be increased. Nevertheless, there is still a great problem when dealing with new coils made from steel with a different chemical composition or with dimensions that have not been previously mapped. CAF control systems face the same problems as other continuous industrial processes in the steel industry, namely, very low flexibility.

1.2 Problem statement

Over the past twenty years, companies have invested to increase their output of galvanised flat steel products to meet an increase in global demand. In addition, today´s markets are rapidly evolving, so production lines have to be adjusted to meet fresh consumer needs in the shortest period of time.

This situation has led galvanising companies to search for greater operational flexibility in production plants. They have started to develop new tools

to allow plant engineers to quickly adjust galvanising lines to new processing conditions.

These tools may be composed of several elements that perform many different tasks such as estimation, control, monitoring, classification, etc. In the galvanising industry, the development of these components is a truly daunting task due to the complexity and inherent nonlinearities of their underlying processes. There exists a general consensus on the need for profound and accurate knowledge on the galvanising process for performing this task.

This knowledge was traditionally found by conducting a number of in-plant process trials, but this is inefficient due to the high costs involved. The most widely used alternative is to use mathematical methods considering the physical properties and mechanics of the process. However, this approach involves great difficulties for swiftly adjusting the component parameters to new product specifications, often requiring high computation time.

The problem addressed in this thesis is the difficulty in making estimates and multiple adjustments for tuning a galvanising line when dealing with new products. One possible approach is to extract the knowledge from the large volumes of data usually captured from the CHDGLs. Most galvanising companies can afford real-time data warehouses or large DBs, but they are unable to take advantage of that "stored knowledge" to save costs.

This challenging problem requires the development of new efficient DM-based methodologies capable of handling large DBs while generating useful knowledge that helps plant engineers to reduce the time required for performing many operational tasks such as estimating optimal set points, explaining failures in the line, scheduling production operations, identifying and classifying product defects during the zinc coating, and so on.

1.3 Scope and Objectives

The scale of data analysis, rule generation and even inferencing in industrial DBs have outrun human capacities. Analysts and plant experts are constantly trying to implement new computer-based methodologies that could be profitably used to extract "process knowledge".

As mentioned above, steel industries need to enhance the flexibility of their key processes to continue being competitive; an in-depth study of their continuous production lines through DM can be extremely useful for tuning the lines´ set parameters, as well as for identifying frequent failures in them.

How to address this need in the galvanising industry by using DM techniques and predictive SC-based modelling is the main scope of this thesis, which has the following five research objectives:

1. specify new semi-automatic methodologies based on DM and SC to obtain knowledge for helping to improve galvanising lines;

2. apply the methodologies proposed in a CHDGL for steel coils, and more specifically to its CAF;

3. evaluate the performance of the methodologies. The proposals will be validated using the data from a CHDGL, whereupon the results detained will be evaluated to decide whether the models developed reflect significant improvements;

4. report a convincing discussion about the knowledge discovered in any of its possible forms, such as rules or overall parsimonious prediction models, and create new opportunities for future developments;

5. hand the knowledge obtained over to operators and plant engineers for its implementation in galvanising plants. This knowledge may be used to automate the tuning of galvanising process that was previously being operated manually.

It should be noted that the validation of the proposals has focused solely on extracting knowledge related to the quality of continuously galvanised coils. However, it is worth mentioning that methodologies of this kind can be used not only for extracting knowledge from this particular industrial process but also extrapolated, with the same potential success, to other fields such as the environment, energy, business, marketing, etc.

1.4 Contributions presented in the thesis

This thesis considers three scientific contributions reported in the following publications referred to by Roman numerals:

Publication I (Martínez-de Pisón *et al.*, 2012). An experience is presented based on the use of association rules from multiple TS captured from a galvanising process, where the main goal is to seek useful knowledge for explaining failures in this process.

An overall methodology is proposed for obtaining the association rules, which represent relations repeated between different pre-defined episodes in multiple TS.

Each episode corresponds to a significant event in the TS, and it is defined within a time window and with a time lag. The initial steps of the proposed methodology involve an iterative, interactive process that involves the use of several pre-processing and segmentation techniques to obtain the significant events in each TS. A search is then made according to a pre-established time window, a time lag, and a pre-set consequent for finding sequences of episodes that are repeated in various TS; lastly, the rules can be extracted for those frequent episodes, i.e. episodes that have a large number of hits.

In our case, this methodology has been applied and validated by extensive experiments using a historical database of 150 variables from a galvanising process for steel coils.

Experiments were designed by Martínez-de-Pisón and all of them were jointly conducted with the auhtos. The author wrote most of the article and Martinez-de-Pisón wrote the other parts of the article.

Publication II (Sanz-García *et al.*, 2012). A methodology is presented for creating parsimonious models to predict set points in production lines. The models generated have lower prediction errors, higher generalisation capacity and less complexity than those generated by a standard method.

The main component of the proposal is a wrapper scheme that includes a multilayer perceptron (MLP) neural network. The number of neurons in the unique hidden layer of the MLP, the inputs selected and the training parameters are optimised to record the fewest errors. The article proposes genetic algorithms (GAs), whereby the wrapper-based scheme is optimised. The optimisation process in-

cludes two fundamental components: a dynamic penalty function to control model complexity and an early stopping criterion (ESC) for interrupting the optimisation phase.

Using the data obtained from the same process as in Publication I, we performed an evaluation comparing our methodology and others previously proposed.

The results show the advantages of our proposal for developing better parsimonious models for predicting temperature set points in industrial processes, and also highlight the potential proposal's range of applicability.

Martínez-de-Pisón provided insight into the theory and helped considerably in the way toward a workable implementation. The author implemented the mxethodology and wrote the article. Furthermore, the author was responsible for planning, conducting, and reporting the experiments.

Publication III (Sanz-García *et al.*, 2013). This paper represents the next step after the work started in Publication II.

Due to the global, evolving nature of the galvanising industry, there is an increasing need to maintain the high quality of products while working with continual changes in the production cycle.

With the aim of achieving better overall models for predicting set points on the CAF, we explore the possibilities of EMs to increase the scope for generalisation and reduce computation costs and the expertise required during training. Three prediction models based on EMs, namely additive regression (AR), bagging (BG) and dagging (DG), are applied to the DB from the same CHDGL used in previous publications. We have developed a comparative evaluation to demonstrate the capacity of proposed EMs to create overall models from industrial databases.

The resulting models perform better in terms of prediction and generalisation capacity without loosing their parsimony, with a significant decrease in the difficulty and cost of setting up the models.

The method was developed by the author. The author designed the experiments, conducted all of them, and wrote the article.

1.4.1 Publications of the thesis

The present thesis consists of an brief introductory part and the following three peer-reviewed publications in two journals listed in the Journal Citation Reports®:

1. Martínez-de-Pisón, F., **Sanz, A.**, Martínez-de-Pisón, E., Jiménez, E. & Conti, D. (2012). Mining association rules from time series to explain failures in a hot-dip galvanising steel line, *Computers & Industrial Engineering* **63**(1), 22-36

2. **Sanz-García, A.** and Fernández-Ceniceros, J. and Fernández-Martínez, R. & Martínez-de-Pisón, F. J. (2012). Methodology based on genetic optimisation to develop overall parsimonious models for predicting temperature settings on an annealing furnace, *Ironmaking & Steelmaking*, *available on line*. DOI 10.1179/1743281212Y.0000000094

3. **Sanz-García, A.** and Antoñanzas-Torres, A. and Fernández-Ceniceros, J. & Martínez-de-Pisón, F. J. (2012). Overall models based on ensemble methods for predicting continuous annealing furnace temperature settings, *Ironmaking & Steelmaking*. DOI 10.1179/1743281213Y.0000000104. *Available on line*

1.4.2 Thematic unit

The framework of three publications informing this thesis involves two main fields: data mining and the galvanising process.

- The first publication (Martínez-de Pisón *et al.*, 2012) focuses on the development and validation of a methodology based on DM for discovering useful knowledge. Specifically, an application based on ARM using a time window and a time lag is proposed to find patterns in TS from an industrial process. The procedure is validated with data collected from a real CHDGL, and it is concluded that the methodology has the capability to extract novel relations between several products and process features.

- The second (Sanz-García *et al.*, 2012) and third (Sanz-García *et al.*, 2013) publications share the implementation of overall parsimonious models for predicting the temperature set points of a CAF on a CHDGL. These contri-

butions provide two methodologies for faciliting the tasks of designing and automatically selecting the best overall parsimonious model.

It is noteworthy that all three methodologies proposed were validated using the historical data from the same CAF on a CHDGL.

1.5 Thesis outline

The document is divided into eight chapters and outlined as follows. Chapter 2 describes previous works on DM and predictive process modelling based on SC for improving industrial processes, focusing especially on industrial applications. Chapter 3, 4 and 5 correspond to the three peer-reviewed publications upon which the thesis is based. Publication I corresponds to research on the field of ARM and the extraction of useful knowledge to explain failures in continuous production lines. Publications II and III both deal with the non-linear modelling of an industrial process using data-driven methods. These publications focus on a particular CHDGL for steel coils, and more specifically on its CAF. In Chapter 6, the findings and results of the three papers are briefly summarised. The general discussion of the thesis continues in Chapter 7, and the conclusions are finally reported in Chapter 8.

Chapter 2

Related Work

This chapter covers recent advances in DM and SC techniques in ironmaking, steelmaking and the manufacturing industry. Representative examples are selected from the numerous industrial applications in which these techniques have been used for knowledge discovering and advanced modelling (Nisbet *et al.*, 2009).

Nowadays, data are captured from industrial processes in many different formats, such as text, numerical values, images, etc. However, according to Hand *et al.* (2001), most of DM techniques focus on dealing with two classes of data: qualitative and quantitative. The former is not so precisely defined and not so specific as the latter. Descriptive techniques are used for working with qualitative data. They are divided into several types depending on the task performed, e.g., ARM is a descriptive technique for discovering relations between items based on hidden patterns. In contrast, quantitative data can be approximated using numerical values. Predictive methods can deal with quantitative data for inferring models of dynamic systems from a series of measurements, taken from these selfsame systems (Norgaard *et al.*, 2003).

In recent years, there seems to have been exponential growth in DM-based applications using both predictive and descriptive techniques in multiple domains. Taken as a whole, both types are able to constitute highly elaborate systems.

In 2009, Choudhary *et al.* reported a full review of several types of DM techniques applied in manufacturing, emphasising on the type of DM function to be performed on industrial data. However, some techniques employed in this

thesis, such as EMs and evolutionary computing (EC), were not included in their review. Complementary information about EMs was provided by Rokach (2009) together with further insight into the vast number of alternatives available. On the other hand, Oduguwa *et al.* (2005) described in detail the status and trends of EC, resolving a wide range of industrial problems.

Recently, Köksal *et al.* (2011) and Liao *et al.* (2012) have presented additional up-to-date reviews describing many applications based on different DM techniques for industry. Although the goals of DM-based applications in the literature are very diverse, two activities are readily apparent: the increase in end-product quality and the inference of non-linear systems for industrial lines. Indeed, these are the main goals of the new methodologies developed in this thesis. For this reason, this chapter is divided in two sectionsaccording to the two types of data that the thesis tackles, i.e. ARM for extracting qualitative data and non-parametric prediction modelling for predicting quantitative data .

2.1 Association rules mining in industrial time series

ARM in TS has generated a considerable interest in many domains in recent years (Core & Goethals, 2010). Seminal works by Das *et al.* (1997, 1998) have highlighted the capability that these techniques have for discovering patterns in multivariate TS, in contrast to traditional analyses that focus largely on global models. For instance, in order to enhance quality control in industry, a growing body of literature has examined the potential of ARM for extracting the hidden knowledge within the TS from their industrial processes (Köksal *et al.*, 2011). Knowledge can be represented as a list of simple rules that would be helpful in decision-making for adopting measures to avoid drops in product quality (Triantaphyllou *et al.*, 2002; Ferreiro *et al.*, 2011).

The basic idea of ARM involves finding frequently-repeated interrelations among multiple TS, and depicting them in a manner that is readily understood by an expert (Haji & Assadi, 2009).

One of the most widely known frameworks for carrying out this task is temporal data mining (TDM). TDM is a set of techniques that extracts valuable information associated with periods of time (Tak-Chung, 2011). According to Abdel-Aal (2008), the interesting feature of TDM is that the presence of the time attribute as a trigger allows more complex patterns to be obtained. These

patterns provide more scope for analysts in terms of understanding and utility, but their proper interpretation usually incurs problems (Zhao & Bhowmick, 2003).

Another basic framework for extracting temporal patterns in TS is the frequent episode discovery framework (Mannila *et al.*, 1997). Generally speaking of thinking, the point of departure for TDM is the work by Mannila *et al.* (1997).

In 2000, Zaki (2000) showed how important it is to use constraints, especially time constraints, in the application of methods to obtain concise results and useful information. Furthermore, in many TS, especially those related to understanding industrial process failures (Shahbaz *et al.*, 2006), the relationships do not occur at the same instant in time, but with time lags. Therefore, the search for events of interest in the antecedent should focus on a time window located before a predefined type of event in the consequent. The development of MOWCATL algorithm by Harms *et al.* (2002) was a significant advance in finding minimal occurrences of episodes and relations between them, which occur within the specified window width. More recently, Huang & Chang (2007) combined the constraints during the discovery process, a time lag between the antecedent and consequent of a discovered rule and relations with episodes from across multiple sequences.

All these publications are closely related to the methodology proposed for ARM in TS. However, in our case the concept of search windows is adopted solely for the antecedent of the rules extracted. It can therefore be said that the constraints on the consequent are increased, given that the desired event is initially known and, what is more, the sole point of interest is the first instant at which it occurs.

In 1994, Agrawal & Srikant defined the ARM in transactional databases (TDBs) by using the APRIORI algorithm. However, the methodology proposed in this thesis for extracting rules focuses primarily on framework proposed by Mannila *et al.* (1997). Hence, mining "episodes" can be considered as our starting point for obtaining temporal relations in a single TS with the aid of a sliding (time) window. The combination of items in a sequence of events gives rise to an episode with a specific order in time. This approach has been applied in many domains, such as assembly lines in manufacturing plants (Laxman *et al.*, 2004), Wal-Mart sales DBs (Atallah *et al.*, 2004), web navigation logs (Casas-Garriga, 2003), and so on.

Other strategies have proven to be even more powerful than the previous ones expressing temporal concepts in interval sequences. In particular, the literature reports certain more complex approaches, such as pattern mining based on Allen's relations (Kam & Fu, 2000), rules expressed with unification-based temporal (UT) grammar (Ultsch, 2004) and temporal rules with the hierarchical time series knowledge representation (TSKR) (Mörchen & Ultsch, 2007). Their use is sometimes not strictly necessary, as the depiction of information can become more difficult to understand, making the pattern space complex for analysts.

The task of extracting minimal occurrences of episodes and relations between them could be accomplished by means of the MINEPI algorithm developed by Mannila *et al.* (1997). Nevertheless, the ECLAT algorithm, proposed by Zaki (2000), is usually used as the support for obtaining frequent item sets in episode DBs. One reason is that ECLAT has proven to be very effective for reducing computation time (Schmidt-Thieme, 2004). This does not mean that ECLAT is the best choice. Indeed, many other algorithms capable of mining for temporal rules in TSDB based on these three methods have been introduced over the past decade. For example, ARMADA (Winarko & Roddick, 2007) and CTMiner(Chen *et al.*, 2010), among others. However, the use of ECLAT does not reduce the degree of generalisation for providing an overall methodology.

The literature reports few applications of ARM for discovering previously unknown rules that enable experts to adopt measures to avoid problems in real industrial processes.

2.2 Non-linear modelling of industrial process

Soft computing attempts to find reasonably useful solutions to complex problems. SC-based methods exploit the tolerance of uncertainty and imprecision to achieve the greater robustness, manageability and lower computation cost of solutions (Zadeh, 1994). The three popular constituents of SC are fuzzy sets, ANNs and GAs (del Jesús *et al.*, 2009).

In recent years, many authors have revealed a growing interest in SC (Argyropoulos, 1990; Schlang *et al.*, 1996, 1999). In 2001, Dote & Ovaska presented a broad review to eliminate the important gap between the theory and practice of these techniques. Choudhary *et al.* (2009) presented a full review of the literature dealing with SC and DM applications in manufacturing domain. In

comparison to this lastest review, other papers focused more on steel processing; so the following paragraphs deal explicitly with the industrial applications of SC techniques.

In 2001, Schlang & Lang presented a number of applications of neural computation for process control in steel processing. Takahashi (2001) described various types of innovations based on Artificial Intelligence (AI) promoted in the field of hot rolling process control. Tang *et al.* (2001) conducted a comparative analysis of certain AI-based planning and scheduling systems for steel production. These papers testify to the considerable amount of literature published on DM and SC applications. However, of all the types of processes associated with industrial domains, those for continuous galvanising and annealing were of particular interest to this thesis.

As mentioned in Chapter 1, CHDGL always includes a CAF upstream of the zinc bath to improve steel properties according to pre-established annealing curves (see Figure 1.4 and Figure 1.5). The annealing treatment of steel coils consists on accurately controlling heating and cooling temperature settings inside a furnace while maintaining the strip velocity within a pre-established range of values. The prediction of CAF temperature settings is an unresolved issue, and several research papers have been published on the use of different approaches for modelling the furnace. The ultimate goal is to enhance the online control of the CAF (Prieto *et al.*, 2005b,a).

Traditional approaches are based on determining temperatures empirically by multiple process trials that create a set of tables (Martínez-De-Pisón, 2003). Today, this inefficient method has been discarded because of the high costs associated with in-plant trials.

A well-known alternative is to develop mathematical models (model-based approach) based on the thermodynamic properties of the furnace materials and the heat transfer mechanics inside the CAF (Jaluria, 1988; Townsend, 1988; 199, 1998; Sahay *et al.*, 2004; Sahay & Kapur, 2007; Mehta & Sahay, 2009). However, as Prieto *et al.* (2005b) contend, some furnace specifications and material properties may change appreciably with different steel compositions and heat treatment, and this may have a significantly bearing on mathematical models.

A further alternative is the development of models based on data (data-based or data-driven approach). They may improve prediction capability because they consider not only the inherent non-linearities of the annealing process

but also the plant operators´ experience and historical data (Tenner *et al.*, 2001; Jones *et al.*, 2005; de Medeiros *et al.*, 2007).

Since 1998, in studies related to regression models, several authors have reported on the use of historical data from steel processes (Yoshitani & Hasegawa, 1998; Schlang *et al.*, 1999), and interest in such models has grown, especially in those based on ANNs (Schlang & Lang, 2001), genetic algorithm guided neural network (GA–NN) ensemble (Yang *et al.*, 2011), fuzzy logic models (Hassan *et al.*, 2012) fuzzy ANNs (Li *et al.*, 2011b), Bayesian models (Agarwal & Shivpuri, 2012), Gaussian mixture models (Yang *et al.*, 2012), among others.

Several applications can readily be found in the literature that apply the fuzzy set theory in CHDGL for system control, quality management, etc. Kuru & Kuru (2011) proposed a new galvannealing control system based on a fuzzy inference system. This system contributed to a significant improvement in the uniformity and quality of the coating layer running at the lower limit of permissible coating values. More recently, Zhang et al. proposed a feed-forward control method based on fuzzy adaptive models for the thickness control process of galvanising coating (Zhang *et al.*, 2012).

In galvanising, Lu & Markward (1997) reported significant improvements using ANNs for coating control. Schiefer *et al.* (1999) presented a combination of clustering and a radial basis function network (RBFN) for improving predictions in the online control of galvannealing process. In 2005, Pernía-Espinoza *et al.* (2005) reported the high performance of robust MLP for estimating the velocity set point of coils inside the CAF using coil specifications and furnace temperatures. Along with this research, other promising papers have developed more reliable models for predicting CAF temperature settings in CHDGL.

In an earlier paper, Martínez-De-Pisón *et al.* (2006) reported a methodology based on combining MLP networks and GAs. Their results showed that correctly tuned MLPs can predict the optimal settings of a CAF control system. Nevertheless, the task of finding the best MLP topology is still a challenging problem. In 2010, Martínez-De-Pisón *et al.* provided support for the use of using MLPs with few hidden neurons instead of more complex networks to produce models with less generalisation error. These models allowed them to predict CAF temperature settings more accurately, in particular dealing with data not previously encountered. Based on previous papers, in 2010 Martínez-De-Pisón *et al.* proposed an overall dynamic model for the strip temperature in the annealing furnace.

The advent of GAs (Mitchell, 1998), which are widely used in many industrial domains (Pal *et al.*, 2006; Pettersson *et al.*, 2009; Yang *et al.*, 2011), has made the task of finding optimal prediction models, especially those based on ANNs, a more tractable problem. GAs are capable of optimising model settings, striking a balance between accuracy and complexity on the one hand, and resources invested in model development on the other. In 2010, Agarwal *et al.* reported on work with evolutionary neural networks to estimate the expected performance of a blast furnace with periodic variations in input parameters and changes in operating conditions. Finally, in 2011, Martínez-De-Pisón *et al.* reported a method based on GAs to find the optimal MLP, with the proposal then being applied to a CAF. This paper enabled satisfactory heat treatments to be given even in cases of sudden changes in strip specifications, such as welding two coils that are totally different in terms of dimensions and chemical composition.

More research into modelling, system identification and control system design is still needed to address the problem of dealing with new steel coils that have not been previously mapped.

Chapter 3

PUBLICATION I

Martínez-de-Pisón, F., Sanz, A., Martínez-de-Pisón, E., Jiménez, E. & Conti, D. (2012). Mining association rules from time series to explain failures in a hot-dip galvanising steel line, *Computers & Industrial Engineering* **63**(1), 22 - 36.DOI 10.1016/j.cie.2012.01.013.

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Mining association rules from time series to explain failures in a hot-dip galvanizing steel line

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ABSTRACT

This paper presents an experience based on the use of association rules from multiple time series captured from industrial processes. The main goal is to seek useful knowledge for explaining failures in these processes. An overall method is developed to obtain association rules that represent the repeated relationships between pre-defined episodes in multiple time series, using a time window and a time lag. First, the process involves working in an iterative and interactive manner with several pre-processing and segmentation algorithms for each kind of time series in order to obtain significant events. In the next step, a search is made for sequences of events called episodes that are repeated among the various time series according to a pre-set consequent, a pre-established time window and a time lag. Extraction is then made of the association rules for those episodes that appear many times and have a high rate of hits. Finally, a case study is described regarding the application of this methodology to a historical database of 150 variables from an industrial process for galvanizing steel coils.

1. Introduction

One of the fields with the brightest future for the quality control of industrial processes corresponds to the search for hidden knowledge within time series (Koskal, Batmaz, & Testik, 2011). Times series may be defined as those stored data that collect information on variables over a period of time, associated with events, patterns or sequences and links for which time is one of the parameters for analysis.

Therefore, time series databases (TSDBs) are now a very useful research tool for obtaining valuable and non-trivial information that can be extracted using temporal data mining (TDM) techniques (Tak-Chung, 2011). Although TDM uses many different methods and applications to handle TSDB, considerable interest has been shown in recent years in the search for associative rules in time series (Core & Goethals, 2010). This interest focuses on the presence of the time attribute as a trigger for obtaining rules and patterns that offer a greater degree of scope for the analyst in terms of understanding, utility and prediction (Abdel-Aal, 2008).

It is well known that the human brain's ability to segment and extract visual patterns is far superior to any existing system of artificial vision. Likewise, the brain is capable of identifying sound, tastes, aromas and textures. The analyst who seeks to extract useful knowledge to improve an industrial process uses this skill to visually discover repetitive events and their relationships over time (Liu & Teng, 2008); to do so, use is made of time graphs like the one shown in Fig. 1.

It often happens that when we hear an expert discuss the behavior of a time series, we hear expressions such as "this segment grows linearly" or "this curve is below a threshold value", which clearly reflect the manner in which human beings locally

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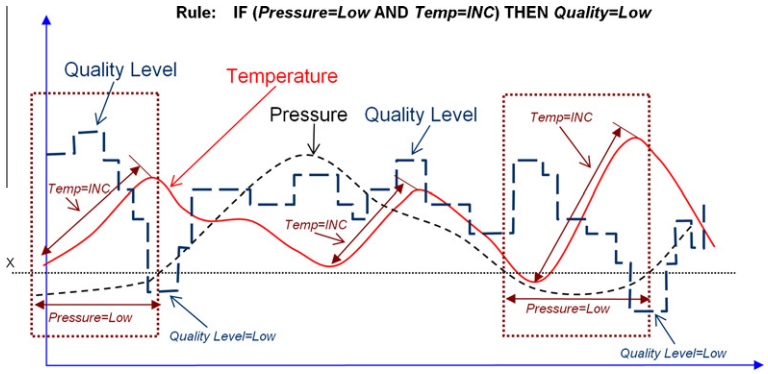


Fig. 1. Detecting time relationships between the variables in an industrial process.

describe a time series. This type of visual segmentation is performed by dividing the time series into segments whose appearance is similar to familiar shapes (lines, rising or falling curves, above or below a value, etc.) just like the way in which the brain describes any new object it encounters (Bishop, 2006; Oliver, Bexter, & Wallace, 1998).

It can be deduced from the above that this task can only be performed visually when the amount of information to be handled is not very great, being practically impossible when the number of variables and readings grows sharply (Gauri & Chakraborty, 2009). This is typical of industrial processes in which we encounter dozens or hundreds of parameters and tens or hundreds of thousands of readings for each one of them (Essafi, Delorme, Dolgui, & Guschinskaya, 2010). Besides, the search for this hidden knowledge may be even further complicated in these cases, as local correlations may not only correspond to the same moment in time, but there may also be dependencies between events with major time lags. This is very common in systems with large inertias, such as certain chemical or physical processes whose response speeds are very slow or even vary according to ambient conditions (Chen & Chai, 2010; Wang, Wang, Du, & Qu, 2003).

This work has focused on developing an overall method to be used for obtaining hidden knowledge, expressed in the form of association rules, from the historical records of complex industrial processes (Chen, Wei, Liu, & Wets, 2002). These rules will be of help in decision-making for improving production processes and adopting measures to avoid drops in product quality (Ferreiro, Sierra, Irigoien, & Gorritxategi, 2011; Triantaphyllou, Liao, & Iyengar, 2002). The basic idea involves finding, amongst multiple time series, interrelations that are frequently repeated and depict these relationships in a manner that is readily understood by an expert (Haji & Assadi, 2009; Ordieres, Martínez-de-Pisón, Castejón, & González, 2005). For example, by analyzing the time series corresponding to a certain industrial process, as shown in Fig. 1, the following rule can be deduced: "when temperature rises and pressure remains below a given level *X*, this leads to a drop in product quality". This previously unknown rule would enable an expert to adopt measures to avoid this drop in product quality.

Specifically, the article describes an experience in a practical case for seeking useful knowledge on a hot-dip galvanizing line (HDGL). This case study has provided knowledge that has been used to identify both the main circumstances that affect the quality of the coating on the coils and the control actions that could be implemented as a safety measure to resolve the problems arising (Alfonso-Cendón, González-Marcos, Castejón-Limas, & Ordieres-Meré, 2010; Martínez-de-Pisón, Ordieres, Pernía, & Alba, 2007).

2. Related work

The issue of locating and acquiring hidden knowledge in large databases has been examined many times in the literature on data mining, and several techniques and applications have been considered (Han & Kamber, 2006; Hand, Mannila, & Smyth, 2001). However, out of all the applications and techniques considered for databases of all types, those for TSDB are of particular interest for current research, as time series can be found in most scientific, financial, meteorological and industrial processes (Dorr & Denton, 2009). The numerous fields and applications that illustrate how TSDB are handled are referred to as temporal data mining (TDM). The surveys by Fu (2011), Laxman and Sastry (2006), Zhao and Bhowmick (2003), for instance, give detailed descriptions of the current topics, scopes and tendencies covered by TDM.

The literature on TSDB reveals that TDM is useful in myriad fields and applications. One of the most productive areas is finance: Last, Klein, and Kandel (2001) investigate stock performance over a 5-year period in series from Standard and Poor's index; Tung, Lu, Han, and Feng (2003) analyze share price movements on the Singapore and Taiwan stock markets; more recently, Huang, Hsu, and Wanga (2007), Huang, Kao, and Sandnes (2008), and Mongkolnavin and Tirapat (2009) extract sequential patterns in the Taiwanese and Thai markets, respectively. Further study areas are environmental science and meteorology: making weather forecasts for Hong Kong (Feng, Dillon, & Liu, 2001), analyzing drought phenomena using oceanic and atmospheric time series (Harms, Li, Goddard, & Waltman, 2003; Harms, Tadesse, Wilhite, Hayes, & Goddard, 2004), or applying correlation studies with time series to ocean systems (Huang, Kao, & Sandnes, 2008).

Closer to our own line of research, applications in industry, quality control and safety systems include Moreno, Ramos, García, and Toro (2008), who use association rules to mine for quality indices in engineering and software projects; Hong, Hong, and So (2009) use temporal rule mining to predict failures in systems for the Korean Air Force; Buddhakulsomsiri and Zakarian (2009) present an algorithm that uses sequential patterns applied to quality assurance systems in the vehicle industry; Lau, Ho, Chu, Ho, and Lee (2009) propose an intelligent quality management system equipped with a new algorithm based on finding fuzzy association rules between process parameters and the presence of quality problems.

For the purposes of this research, a basic data mining framework applied to TSDB in just two items is developed by Last (2004): (Phase: 1) pre-processing and segmentation of time series; and (Phase: 2) subsequent extraction of temporal relationships between the items in the databases. This research framework has been adopted as the script for the study made here.

Focusing explicitly on the first phase, numerical time series are often converted to event sequences by segmentation (Last et al., 2001; Terzi & Tsaparas, 2006; Keogh, Chu, Hart, & Pazzani, 2004), cluster analysis (Bellazi, Larizza, Magni, & Bellazi, 2005), or discretization (Mörchen, Ultsch, & Hoos, 2004). There are numerous methods that produce different types of discrete-time data series, whereby data mining methods tend to study and explore different possibilities. The characteristic patterns or events extracted are capable of providing the necessary information regarding the behavior of the time series, even in the case of anomalous circumstances.

The second phase of the data mining framework presented by Last (2004) points out that TSDB can be transformed into transactional databases with an added time dimension, which by extrapolation can be treated according to classical association rules and frequent itemset (occurrences) searches along with the time parameter. The following paragraph analyzes different studies based on this line of research, converting the time series to event, episode, or interval sequences. Other studies, such as the inter-transactional approach (Dong, Li, & Shi, 2004; Tung, Lu, Han, & Feng, 1999, 2003), are not considered in this work. In this particular instance, it seeks to mine for temporal rules looking first for transactional rules and then extrapolates the subset obtained to an inter-transactional approach.

The point of departure for this study stems from the work by Mannila, Toivonen, and Verkamo (1997), although associative rule mining in transactional databases is introduced by Agrawal and Srikant (1994) using the APRIORI algorithm. Mannila et al. (1997) illustrate the mining "episodes" as a starting point for obtaining temporal relationships in single time series with the aid of a sliding (time) window. The combination of items in a sequence of events gives rise to an episode given a specific order in time. By means of the MINEPI algorithm (introduced by Mannila) minimal occurrences of episodes and relationships between them are extracted. Das, Gunopulos, and Mannila (1997), Das, Lin, Mannila, Renganathan, and Smyth (1998) subsequently highlight the discovery of patterns in multivariate time series, in contrast to traditional time series analysis which largely focuses on global models. Similarly, Bettini et al. (1996, 1998) propose the use of event structures, which consist of a number of variables that represent events and time constraints between them, for bringing to light temporal relationships between events in an episodal sequence.

Subsequent research (Zaki, 2000) has shown how important it is to use constraints (especially time constraints) to obtain more concise results and useful information. Consequently, algorithms such as Gen-FCE and Gen-REAR (Harms, Deogun, Saquer, & Tadesse, 2001) propose the extraction of minimal occurrences of episodes and relationships between them using constraints for discovering representative episodal association rules (REAR). This latter method is designed solely to close frequent episodes and it is impossible to find interesting patterns with a relatively low frequency in the database.

Furthermore, in many time series, especially those related to understanding industrial process failures, the relationships do not occur at the same instant in time, but instead record time lags. Therefore, the search for events of interest in the antecedent should focus on a time window located before a pre-defined type of event in the consequent. The MOWCATL algorithm (Harms, Deogun, & Tadesse, 2002) finds minimal occurrences of episodes and relationships between them, which occur within the specified window width. This approach uses constraints during the discovery process, a time lag between the antecedent and consequent of a discovered rule, and relationships with episodes from across multiple sequences.

More recently, Huang & Chang, 2007 extend the MINEPI algorithm to both MINEPI + and EMMA for mining frequent episodes in complex sequences that consist of a set of events at each time slot in terms of various intervals (hours, days, etc.).

This research has adopted the concept of search windows only for the antecedent. The constraints on the consequent are increased, given that the desired episode is initially known and, what is more, the sole point of interest is the first instant at which it occurs.

Another well-known algorithm, ECLAT (Zaki, 2000), is particularly significant for this research, proving to be very effective in reducing computation times (Schmidt-Thieme, 2004) and being used as a support for obtaining frequent itemsets in the episode database.

Finally, there are other approaches, such as those by Last et al. (2001) and Villafane, Hua, Tran, and Maulik (2000), which propose procedures to discover containments of intervals or successive intervals to gain insight into the temporal relationships across various events. Other subsequent methods are even more powerful than the previous techniques to express temporal concepts in interval sequences: patterns based on Allen's relations (Kam & Fu, 2000), rules expressed with Unification-based Temporal Grammar (Ultsch, 2004) and temporal rules with the hierarchical language called Time Series Knowledge Representation (Mörchen & Ultsch, 2007). Several algorithms capable of mining for temporal rules in TSDB based on these three methods have been introduced: ARMADA (Winarko & Roddick, 2007) and CTMiner (Chen, Jiang, Peng, & Lee, 2010), amongst others. In our view, they are not strictly necessary for this work, as the depiction of information can become more ambiguous, making the pattern space complex for analysts.

3. Material and methods

The method begins by pre-processing and segmenting time series in order to obtain useful events (Dasha, Nayaka, Senapatia, & Lee, 2007). Due to the broad heterogeneity of the various types of time series underpinning industrial processes (temperatures, pressures, etc.), experts must work in an iterative and interactive manner with several pre-processing and segmentation algorithms for each kind of time series in order to obtain significant events (Gauri & Chakraborty, 2006).

Once the characteristic events have been detected, an essential requirement for establishing a possible relationship is the presence of ordered sequences, called episodes, in which the same combination of events always appears. Informally, a partially ordered collection of events occurring together is defined as an episode (Mannila et al., 1997). For example, in the case of Fig. 1, temperature should rise linearly, pressure should remain below a certain level and product quality should drop, with this occurring on a significant number of occasions within an appropriate time window.

In the next stage, a search is made for episodes that are repeated among the various event sequences according to the pre-established consequent, time window and time lag. The goal is to analyze all event sequences to discover frequent episodes.

Finally, the association rules for those episodes that appear on many occasions and have a high rate of hits are extracted. Association rules are sentences of type $X \Rightarrow Y$ (X implies Y, X called the antecedent and Y the consequent), where X, Y are sets of frequent items in a given database whereby $X \cap Y = \emptyset$. The rule has support and confidence values which can be described as follows:

$$Support\ (X \Rightarrow Y) = P(X \cup Y) \tag{1}$$

$$Confidence\ (X \Rightarrow Y) = P(Y|X) \tag{2}$$

where the support for the rule (Eq. (1)) represents the percentage of transactions in the database that contain both X and Y, and the confidence for the rule (Eq. (2)) is the percentage of transactions in the database containing X that also contain Y. This rule will be

interesting if it has high support and confidence values, which are usually greater than a user's defined threshold values.

The overall method comprises the following stages:

1. Filtering each time series to eliminate noise and obtain its basic form.
2. Obtaining important minima and maxima.
3. Extracting the characteristic events of each time series.
4. Grouping events into episodes according to expert criteria.
5. Creating the episode database T according to time constraints.
6. Searching for association rules with minimum support and a user-defined consequent.

3.1. Step 1: Filtering each time series to eliminate noise and obtain its basic form

A time series may have different spurious values, noise from diverse sources, missing values, etc. which have to be eliminated or reduced by means of different filtering strategies. This first step is crucial to the success of the subsequent stages in knowledge discovery in databases (KDD).

In practice it is observed that, in the event of a wide variety of types of time series, filtering cannot be automatic and clearly depends on an exploratory process for selecting the best filters for each time series recorded.

Iterative software called CONOTOOL was used to facilitate the analysts' task in this critical process. This application enables numerous filters to be applied sequentially to each time series (Fig. 2). Some of these filters are:

1. Sliding-window filters with different functions: Gaussian, rectangular, maximum, minimum, median, etc. These filters are useful for smoothing the time series, and the most important parameter in samples is the width of the discrete-time window. The wider the window, the smoother the original series will be.
2. Filters which use a threshold value (according to a minimum or maximum value or within a range) to eliminate spurious data. Filters of this kind use the last valid value appearing at instant $t-1$ to replace the values for instant t that are above or below a threshold set by the user.
3. Filters based on the Fast Fourier Transform (FFT) to remove high or low frequency harmonics. With this type of filters, the expert specifies the range of frequencies to be discarded.

Using CONOTOOL software, users can apply different filters to each time series. In this manner, the effect of a single filter on the time series can be called up with the "*Plot*" button, or the impact of a series of filters applied to it can be displayed using "*Apply all filters to this Attribute*" button. The original series appears in black and the filtered series in red. The order of application of the filters is chosen according to the order in which they appear on the screen (top-down). Clicking on the buttons up, down, delete, etc. allows conveniently reorganizing the filter bank.

Accordingly, researchers select and adjust the filters for each time series in order to obtain the basic form of the series. This is a necessary step prior to the next stage of the proposed method (Step 2), which involves the search for the most important minima and maxima.

3.2. Step 2: Obtaining important minima and maxima

Once the signal has been filtered, important minima and maxima are obtained for each time series in order to identify increasing, horizontal and decreasing events. The aim is to discard minor fluctuations and keep important minima and maxima.

The technique was extracted from (Fink & Pratt, 2004). A point a_m of a series $\{a_1, \ldots, a_n\}$ is considered an important minimum if there are indices i and j such that:

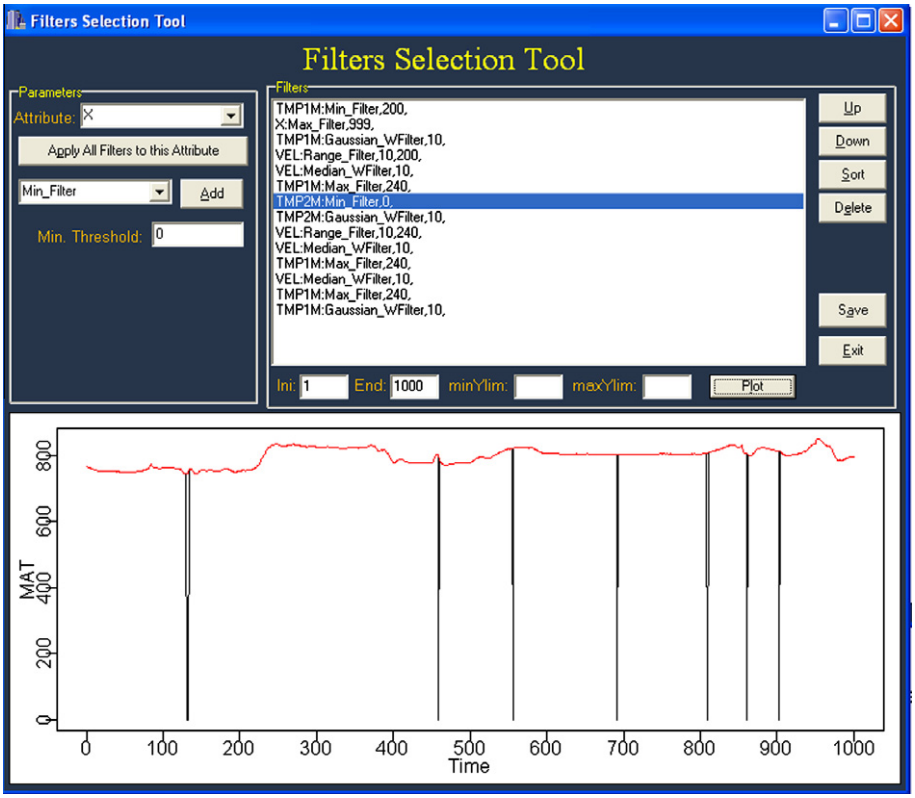


Fig. 2. Example of using CONOTOOL to remove low outliers in a temperature time series.

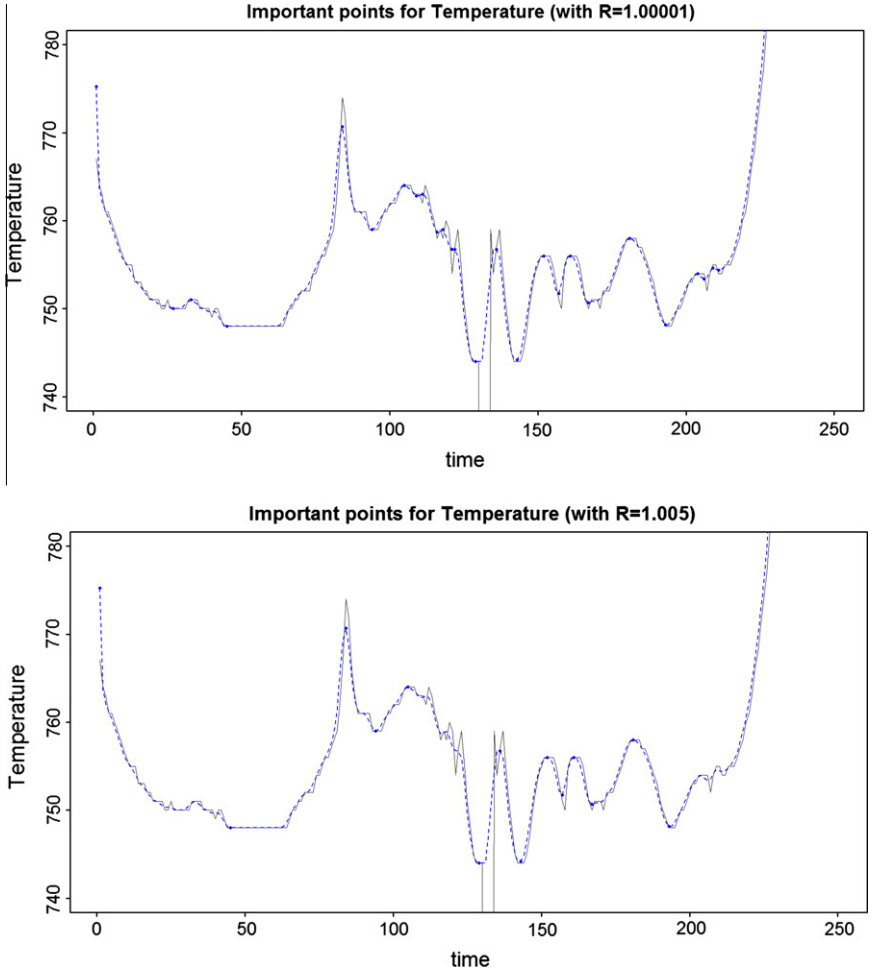


Fig. 3. Example of filtering a temperature and detecting minima and maxima with $R = 1.00001$ and $R = 1.005$ of the final filtered temperature (black solid line = original temperature; blue dashed line = filtered temperature).

$$\begin{cases} a_m \text{ is mininum among } a_i, \ldots, a_j, \text{ and} \\ \frac{a_i}{a_m} \geq R \text{AND } \frac{a_j}{a_m} \geq R \text{ (where, } i \leq m \leq j) \end{cases} \quad (3)$$

and similarly, a_m as an important maximum if:

$$\begin{cases} a_m \text{ is a maximum among } a_i, \ldots, a_j, \text{ and} \\ \frac{a_i}{a_m} \geq R \text{AND} \frac{a_j}{a_m} \geq R \text{ (where, } i \leq m \leq j) \end{cases} \quad (4)$$

where R is a (compression) rate which is always greater than one.

The procedure for selecting important minima and maxima is based on the search for the value of R that allows identifying useful points. Researchers therefore rely on their experience to decide which ones may be useful for estimating the characteristic events to be looked for at this stage of the method (Step 3). The value of R needs to be adjusted for each time series in an iterative way until the appropriate minima and maxima are achieved. This value will always be greater than 1.0. Values of R close to 1.0 will produce too many maxima and minima, many of which are not required. Values further away from 1.0 will produce very few maxima and minima.

Fig. 3 shows an example of the detection of the maximum and minimum values of a temperature variable with $R = 1.00001$ and $R = 1.005$. In the first case ($R = 1.00001$) it can be seen that there are too many maxima and minima, whereas in the second case ($R = 1.005$), the number of maxima and minima is reduced to an acceptable level.

In this second step, there is also a need to perform an iterative process to visually determine the most useful values of R for each time series. Regarding the example in Fig. 3, it is worth noting that the original temperature (black continuous line) has first been filtered to eliminate the low spurious data due to failures in the acquisition system, whereupon application has been made of a Gaussian filter involving a window with a width of five samples in order to smooth the shape of the definitive signal (blue[6] dashed line).

3.3. Step 3: Extracting the characteristic events of each time series

The principal aim in this step is to identify events in each time series according to the height (on the Y coordinate), width (on the X coordinate) and type of curve as per values established previously by the analyst for each time series.

Fig. 4 shows user parameters, conditions and a visual interpretation for each type of event proposed. Fig. 5 presents examples of the extraction of DEC and INC events from a temperature variable. Fig. 6 shows the CONOTOOL window used to define the event search according to Fig. 4 parameters.

A possible event set in the study could be $I' = \{INC, DEC, HOR, OVER, BELOW, BETWEEN\}$. Yet in addition to the possible events in I', there is an added option of using the operator NOT for events that do not fulfill a certain condition. For example, a NOT_BETWEEN event may correspond to those parts of the series that do not fall between two pre-defined threshold values. Such is the case of a

[6] For interpretation of color in Figs. 1–7 and 10, the reader is referred to the web version of this article.

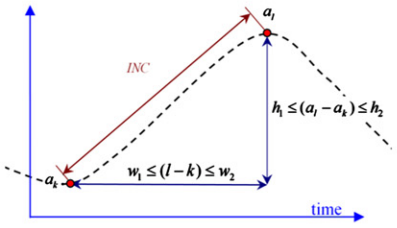
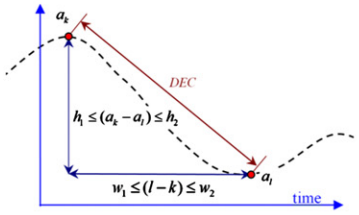
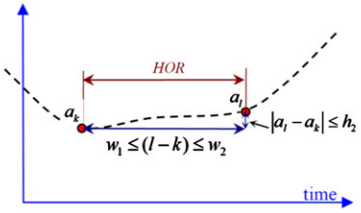
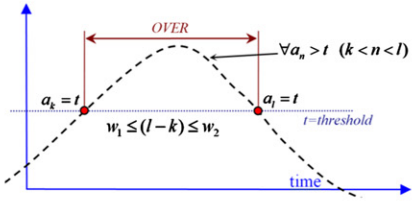
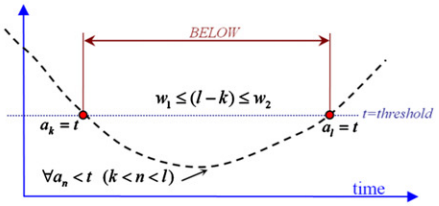
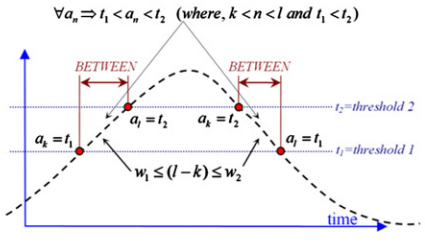
Type	User parameters	Conditions	Visual interpretation
Incremental Event (INC)	$\{w_1, w_2\}$ = Range of X within which the curve is to be contained. $\{h_1, h_2\}$ = Range of Y within which the curve is to be contained.	a_k is a minimum a_l is a maximum $w_1 \le (l-k) \le w_2$ $h_1 \le a_l - a_k \le h_2$	
Decremental Event (DEC)	$\{w_1, w_2\}$ = Range of X within which the curve is to be contained. $\{h_1, h_2\}$ = Range of Y within which the curve is to be contained.	a_k is a maximum a_l is a minimum $w_1 \le (l-k) \le w_2$ $h_1 \le a_k - a_l \le h_2$	
Horizontal Event (HOR)	$\{w_1, w_2\}$ = Range of X within which the curve is to be contained. $\{0, h_2\}$ = Range of Y within which the curve is to be contained.	a_k and a_l are important points $w_1 \le (l-k) \le w_2$ $\lvert a_l - a_k \rvert \le h_2$	
Event over a threshold (OVER)	$\{w_1, w_2\}$ = Range of X within which the curve is to be contained. t = Threshold value.	$a_k = t$ $a_l = t$ $w_1 \le (l-k) \le w_2$ $\forall a_n > t \quad (k < n < l)$	
Event below a threshold (BELOW)	$\{w_1, w_2\}$ = Range of X within which the curve is to be contained. t = Threshold value.	$a_k = t$ $a_l = t$ $w_1 \le (l-k) \le w_2$ $\forall a_n < t \quad (k < n < l)$	
Event between two thresholds (BETWEEN)	$\{w_1, w_2\}$ = Range of X within which the curve is to be contained. t_1 = Min. threshold value. t_2 = Max. threshold value.	$a_k = t$ $a_l = t$ $w_1 \le (l-k) \le w_2$ $\forall a_n \Rightarrow t_1 < a_n < t_2$ (where, $k < n < l$)	

Fig. 4. Parameters, conditions and visual interpretation for each type of event.

series of temperatures in which the lower and upper thresholds are set at 300 °C and 600 °C, respectively. A NOT_BETWEEN event is generated when the temperature exceeds 600 °C or drops below 300 °C. Likewise, a NOT_HOR event can be generated when the time series is not horizontal. Therefore, the final event set in the study is $I = \{INC, DEC, HOR, OVER, BELOW, BETWEEN, NOT\_HOR, NOT\_BETWEEN\}$.

Formally, given a set $I = \{I_j, j = 1, \ldots, m\}$ of event types, an event e (Mannila et al., 1997) is defined as a pair (A, t), where $A \in I$ is an event type and t is an integer, the (occurrence) time of the event. In this work, A is considered to be a single attribute. For example, as shown in Fig. 7, events can be $(I1, 3)$, $(I2, 8)$, $(QLow, 22)\ldots$

We formulate an event sequence S on I as a triple (s, T_s, T_e), where $s = \{(A_1, t_1), (A_2, t_2), \ldots, (A_n, t_n)\} = \{e_1, e_2, \ldots, e_n\}$ is an ordered sequence of events e_i such that $A_i \in I$ for all $i = 1, \ldots, n$, and $t_i \leqslant t_{i+1}$ for all $i = 1, \ldots, n-1$; and T_s and T_e are integers: T_s is called the starting time and T_e the ending time, and $T_s \leqslant t_i < T_e$ for all $i = 1, \ldots, n$. For example, as shown in Fig. 7, an event sequence

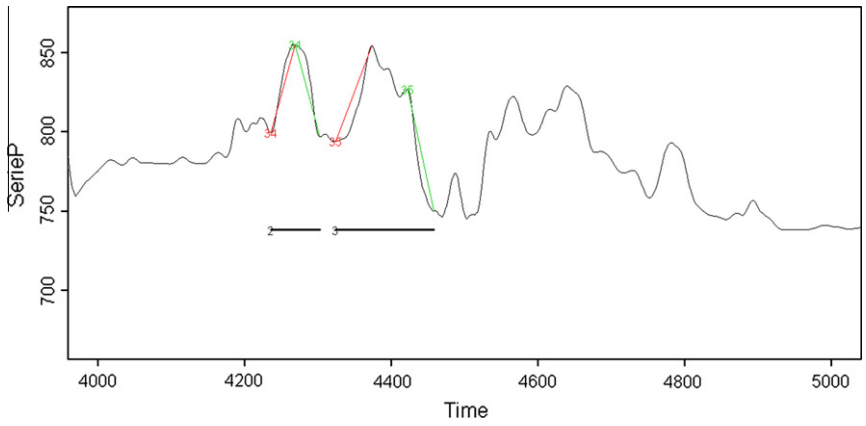


Fig. 5. Extraction of two patterns consisting of an INC event followed by a DEC one.

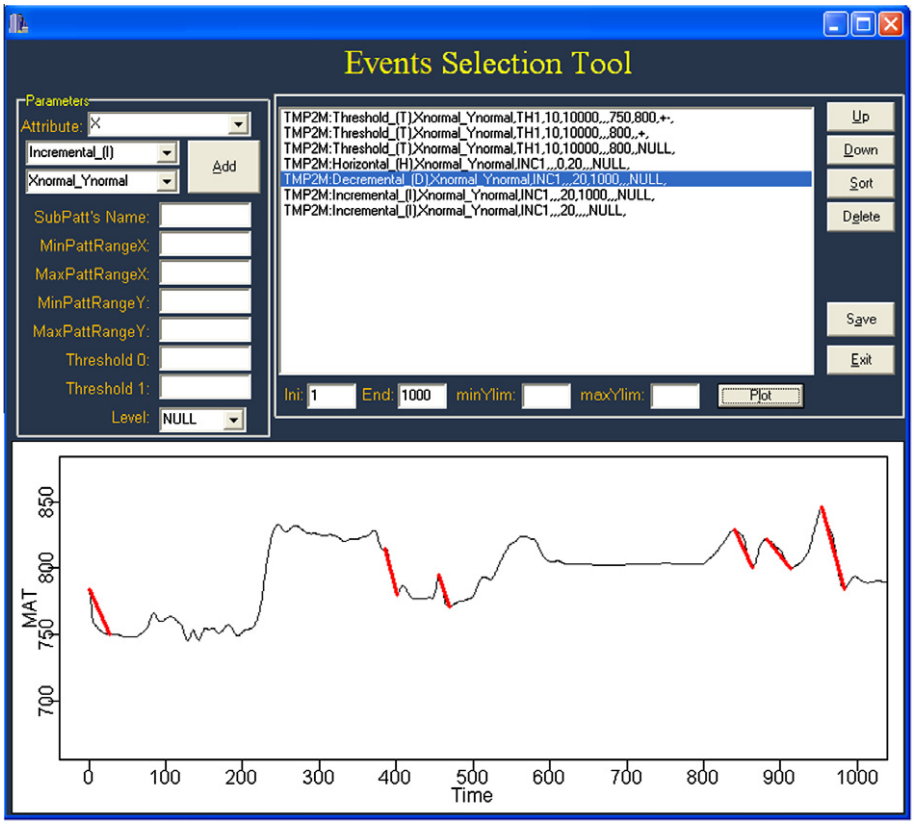


Fig. 6. Example of searching decremental events with CONOTOOL.

can be $\{(I1,3),(I1,4),(I1,5),(I1,6),(I1,7),(I3,7),(I1,8),(I3,8)\ldots,(I2,16),T_s=2,T_e=16\}$.

It is evident that the event search process depends both on obtaining the appropriate maxima and minima in the prior stage (Step 2) and on ensuring the expert's search criterion is the right one in Step 3.

3.4. Step 4: Grouping events into episodes according to expert criteria

Once the important events have been obtained for each time series, it is then possible to search for a combination of several of them. The idea is to define the sequence of events called an episode to be found within a window defined by the user.

An episode α (Mannila et al., 1997) is a triple $(V,\leqslant,g)$ where V is a set of nodes, $\leqslant$ is a partial order on V, and $g: V \to I$ is a mapping that associates each node with an event type. The interpretation of an episode is that the events in $g(V)$ have to occur in the order specified by $\leqslant$. An episode $\alpha=(V,\leqslant,g)$ therefore occurs in an event sequence $S=(\{(A_1,t_1),(A_2,t_2),\ldots,(A_n,t_n)\},T_s,T_e)$ if there is an injective mapping $h: V \to \{1,\ldots,n\}$ from nodes α to events S, such that $g(x)=A_{h(x)}$ for all $x \in V$. For example, as shown in Fig. 7, an episode can be $\langle(I1,8),(I3,7),(I2,14)\rangle$ in a previous event sequence it can be $\{(I1,3),(I1,4),(I1,5),(I1,6),(I1,7),(I3,7),(I1,8),(I3,8)\ldots,(I2,16),T_s=2,T_e=16\}$.

Episodes can be serial, parallel, and non-serial and non-parallel, as shown by Su (2010). A parallel episode is defined without constraints on the order of two events. A serial episode is when

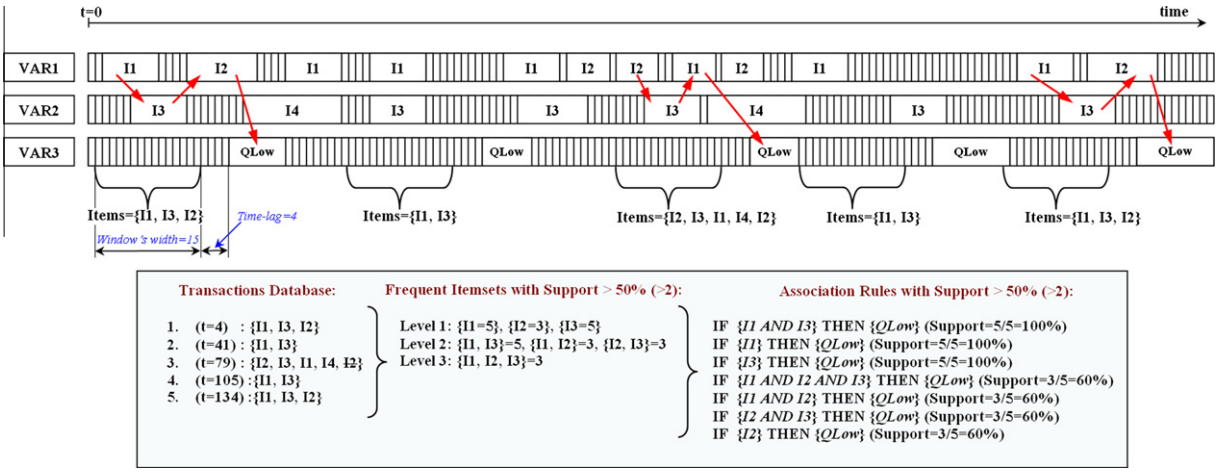


Fig. 7. Example of search for association rules in three time series with *RelSupportWinRule* > 50%, consequent = (QLoW), window width = 15 and time-lag = 4.

the events have to occur in a pre-defined order. Lastly, a non-serial and non-parallel serial episode occurs if there are occurrences of two events and these precede an occurrence of a third event, but no constraints are made on the relative order of the first events. This paper uses only serial episodes.

The method makes flexible searches by combining an asterisk with events. For example, there is the following search:

$$\textit{Window width} = 300 : \langle e_1 = (\textit{TEMP\_INC}^*), \quad e_2 = (*), e_3 = (\textit{PRES\_OVER})\rangle$$

This will search, within a time window of 300 units of time, for those episodes with a first event whose label begins with "*TEMP_INC*", as an event corresponding to a fast temperature increase, the second event can be anything or nothing and the third event is (*PRES_OVER*). The position of the episode found can be stored in a database with the name specified by the user, along with position and length.

From here on, each episode α is considered an itemset in an event sequence *S*.

3.5. Step 5: Creating the episode database T according to time constraints

This step seeks to create the database *T* from which association rules can be obtained (*Step 6*). *T* is generated with the episodes (itemsets) that appear together in a window prior to the consequent (Fig. 7). In this case, ECLAT algorithm (Zaki, 2000) will be used to find the frequent itemsets required for extracting the rules of association.

In this way, the algorithm seeks out frequent episodes that appear within a pre-set sliding time window *W* before the appearance of a consequent set by the analyst. The lag *TimeLag* between the window *W* and the consequent is also set by the user. Setting the consequent of the rule as, for instance, an event concerned with loss of quality or the appearance of a certain defect simplifies and speeds up the search process. In Step 5, each transaction is made up of the episodes that appear before a pre-set consequent, within a time window *W* with a set width *WinW* and a lag *TimeLag* also set by the analyst.

Fig. 7 shows an example of the creation of a transactional database *T* and the search for rules that exceed the minimum support value (Steps 5 and 6). In this case rules are sought within three time series with a *RelSupportWinRule* of more than 50% and the consequent equal to low quality (*QLow*); the window width *WinW* is 15 units of time (ut) and the time lag *TimeLag* is 4 ut, i.e. the antecedent *X* occurs 4 ut before the consequent *Y*, and the items in it appear within a range of $|X_{tot}|$ 15 ut. The final database comprises five transactions, corresponding to the number of appearances of the consequent (*QLow*). The third transaction shows that event (*I2*) is repeated, but only one appearance is taken into account because the initial objective is to locate the appearance of a type of event in an antecedent, regardless of how many times and in what order it appears.

This database is used to determine the frequent itemsets whose supports are higher than the threshold value set and the support and confidence values of the association rules obtained.

The notation used in the algorithm and steps is presented below.

Notation

WinW	Window width (in units of time, ut)
TimeLag	Rule time-lag (ut)
Conseq	Consequent
E	Event sequence database
$\|E\|$	Number of items of E
$e_i(attrib, pos)$	Event where $i = 1,\ldots,n$; attrib = item name; pos = item position
E_{order}	Database E ordered by e_i(attrib, pos)
T	Transactional episode database. Each item $tr_j = \langle T_s, T_e, E_k\rangle$ where T_s and T_e represent the start and the end of transaction
t.count	Transaction counter

Steps of the algorithm

Step 5.1: Define *Win W*, *Time Lag* and *Conseq*. Initialize *t.count* = 0.

Step 5.2: For $i = 1$ to $|E|$ If $(e_i(attrib, pos) \in E_{order} = Conseq)$ Set $T_s = pos - WinW - TimeLag$; $T_e = pos - TimeLag$; Extract E_k as a subset of items $e_j(attrib, pos) \in E_{order}$ where $(T_s \leqslant pos \leqslant T_e)$, $\forall e_j \in E_k$; Delete equal items of E_k; Creates new $tr_{tcount} = \langle T_s, T_e, E_k\rangle$; Set *t.count* = *t.count* = +1; End

3.6. Step 6: Searching for association rules with minimum support and a user-defined consequent

An association rule according to time constraints is defined as:

$$XY \Rightarrow \quad [WinW, TimeLag] \tag{5}$$

which corresponds to an antecedent *X* which occurs at a *TimeLag* before consequent *Y* within a time window of width *WinW*, and where:

$$\textit{RelSupportWinRule} = |X|/|Y| \tag{6}$$

$$RelConfidenceWinRule = |X|/|X_{tot}| \quad (7)$$

with $|Y|$ being the number of times the consequent appears, which is equal to the number of transactions of database T and $|X|$ being the number of times the frequent itemset X appears in T and $|X_{tot}|$ being the number of times X appears in the time and within a time window of width *WinW*. Therefore, *RelSupportWinRule* shows the percentage of times X has occurred when Y has occurred, while *RelConfidenceWinRule* shows the percentage of times the rule has occurred when X has occurred.

For instance, as shown in Fig. 7, for the rule "*IF* {(*I1*) *AND* (*I2*) *AND* (*I3*)} *THEN* {(*QLow*)}" it is determined that the frequency of the consequent is $|Y = 5|$, the frequency of the antecedent when the consequent appears is $|X| = 3$ and the frequency of the antecedent throughout the database using a window width of 15 is $|X_{tot} = 4|$. Thus, the relative support value and the relative confidence value are $ResSupporWinRule = \frac{|X|}{|Y|} = \frac{3}{5} = 60\%$ $RelConfidence WinRule = \frac{|X|}{|X_{tot}|} = \frac{3}{4} = 75\%$.

The search for frequent itemsets in database T that exceed the minimum support defined by the analyst *MinSupport* is conducted using the well-known ECLAT algorithm (Zaki, 2000). Once each antecedent X has been determined, $|X_{tot}|$ is calculated by a sequential search through the whole database of items, using a window of width *WinW*. From these values it is easy to obtain other metric values for predetermining the degree of significance of the rule obtained, although it should be noted that the calculations are relative to the number of times that consequent Y or antecedent X occur in a window of width *WinW*, i.e. $|Y|$ and $|X_{tot}|$ respectively, and not relative to the number of items in database T.

The notation used in the algorithm and steps is presented below.

Notation

MinSupport	Minimum rule support threshold in percentage
MinConfidence	Minimum rule confidence threshold in percentage
WinW	Window width (ut)
TimeLag	Window time-lag (ut)
Conseq	Consequent
T	Transactional episode database obtained from Step 5
$\|T\|$	Number of episodes of T
E	Event sequence database
$\|E\|$	Number of items of E
$e_i(attrib, pos)$	Event where $i = 1,\ldots, n$; attrib = item name; pos = item position $E_{order;}$ Database E ordered by e_i(attrib, pos)
L_k	L_k is the k-frequent itemset from T with L_j(Support) $\geqslant$ MinSupport
$L_k(Support)$	Percentage of L_k that appears in the T database
$\|L_k(Support)\|$	Number of times that L_k appears in the T database
$\|L_k(Count)\|$	Number of times that L_k appears in a window with width WinW
$\bigcup_k L_k$	Database of L_k

Steps of the algorithm

Step 6.1: Define *MinSupport*, *MinConfidence*, *WinW*, *TimeLag* **and** *Conseq*.

Step 6.2: Calculate *MinSupItemset* = *MinSupport*$|T|$

Step 6.3:Use **ECLAT** algorithm to obtain $\cup_k L_k$ from T where L_k is the k-frequent itemset with $L_k(Support) \geqslant MinSupItemset$

Step 6.4:For each L_k from $\cup_k L_k$ then $|L_k(Count)| = 0$; Set $T_s = 0$; $T_e = WinW$; While $(T_e \leqslant pos_{e_n})$Extract G_k as a subset of items $g_j \in E_{order}$ where $(T_s \leqslant g_j(pos) \leqslant T_e), \forall g_j \in E_k$; If $(L_k \subseteq G_k)$ Set $|L_k(Count)| = |(Count)| + 1$; $T_s = T_s + WinW$; $T_e = T_e + WinW$; or else Set $T_s = T_s + 1$; $T_e = T_e + 1$; End End.

Step 6.5:For each L_k from $\cup_k L_k$ then

Calculate and Save $RelSupportWinRule = |L_k(Support)|/|Y|$ and $RelConfidenceWinRule = |L_k(Support)|/|L_k(Count)|$; End.

Step 6.6:Report rules, order by *Relsupport WinRule*, whose *RelSupport WinRule*and *RelConfience WinRule*are higher than the threshold values *MinSupport* and *MinConfidence* defined by the user.

4. Case study: Extracting rules from a HDGL

The presentation is made here of an application of these techniques involving the search for the causes of losses of quality in the coating of new steels at a galvanizing plant. The study provided knowledge that was used to identify the circumstances affecting the quality of the coating on the coils. In particular, the aim was to identify the impact of galvanizing process parameters on the adherence of the zinc coating, which is one of the key factors in the galvanized product's resistance to corrosion.

4.1. Description of the problem

Resistance to corrosion tends to depend on the quality, thickness and uniformity of the zinc coating, being affected by numerous factors (Dobrzanski, Kowalski, & Madejski, 2005; Martínez-de-Pisón, Alba, Castejón, & González, 2006; Martínez-de-Pisón et al., 2007), such as the priming of the metal surface, the composition and temperature of the zinc bath, speed of the strip, control of the air-knives that regulate the thickness of the coating, temperature of the strip, quality of the annealing cycle, and composition of the atmosphere. There should be a minimal or zero content of oxygen in each one of the process stages so as to avoid oxidation.

The adjustment of all the parameters corresponding to each kind of coil according to the type of steel and its dimensions (thickness and width) is a highly laborious task. In addition, such problems are further aggravated when the process involves new steels or new thicknesses that have not been processed before and for which no accurate information or suitable mathematical models are available.

When dealing with these new products, the plant engineers have to make estimates and multiple adjustments until they achieve the right adherence and uniformity for the zinc coating. This involves a great deal of time and wasted material.

It often happens that the implicit knowledge generated by this work is not recorded anywhere, as the large number of variables to be modified and adjusted renders it is extremely difficult to decide which ones are crucial to the quality of the end product.

It is not an easy problem to solve, for in addition to the vast number of variables with a bearing on the process, the number of faulted coils recorded in the databases to be analyzed is not usually very high, thereby considerably hindering the analysis using standard techniques of multivariate statistics (Ordieres-Meré, Martínez-de-Pisón-Ascacíbar, González-Marcos, & Ortiz-Marcos, 2008; Pernía-Espinoza, Castejón-Limas, González-Marcos, & Lobato-Rubio, 2005).

4.2. Description of the industrial process

In general terms, the process involving a continuous HDGL can be described as follows (Fig. 8):

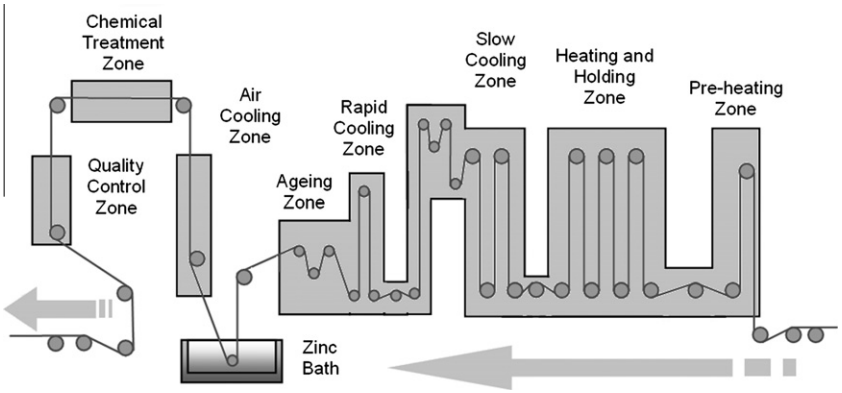


Fig. 8. Basic diagram of a hot-dip galvanizing line.

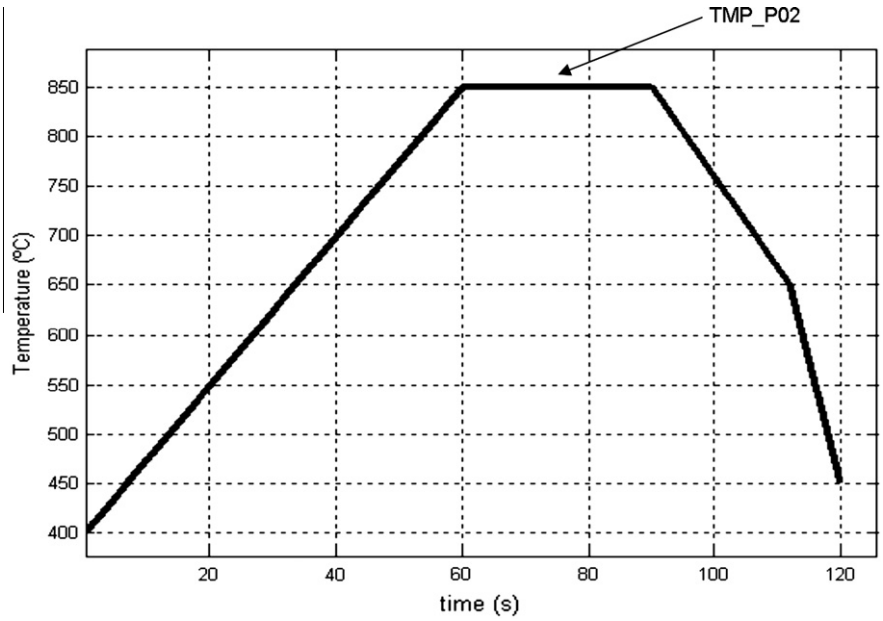


Fig. 9. Example of thermal treatment curve in the annealing phase.

1. The first step consists in forming a continuous strip from the steel coils from the rolling mill. This involves cropping the head and tail of t he same and lap welding them. The end result is a continuous strip of steel formed by the incoming coils.
2. The strip then passes through a pre-heating area in a non-oxidizing atmosphere in which impurities are removed, rolling oils are volatized and surface oxide is reduced.
3. The strip is subsequently subjected to a heating and cooling cycle that is called "annealing" (Fig. 9). This process is essential for improving the properties of the steel and final coating. The aim is to recrystallise the tempered steel from the cold rolling and consolidate the crystalline structure.
4. The furnace in which this process takes place is usually divided into several areas: a heating zone consisting of eight sub-zones, a holding zone, a slow cooling zone and a rapid cooling zone. After rapid cooling, there is an aging or "equalizing" process for ensuring carbon precipitation, and thereby minimizing the effects of steel aging.
5. The strip is then submerged in a pot of molten zinc at constant temperature for the corresponding coating. The strip leaves this bath vertically and passes through air-knives that regulate the thickness of the coating.
6. It then undergoes a series of ancillary processes involving chemical treatments in which a thin film of chromic acid is applied to prevent soft oxidation.
7. Finally, it is flattened to produce the end product in the form of either coils or cut sheets.

This description, albeit with minor modifications, generally applies to the majority of continuous galvanizing lines by immersion operating throughout the world.

The study involved a batch of 723 coils of a new type of steel in which 5.4% (39) of them recorded irregularities in the adherence of the zinc layer. The database was based on the first adjustment tests at the plant, whereby there was a relatively significant percentage of coils with uneven adherence.

4.3. Time series selection

The first step was to select the variables that could have the most influence on the galvanizing process (Dobrzanski et al., 2005; Martínez-de-Pisón et al., 2007). The variables were selected with the help of the plant's technicians. In addition, referral was made to the studies conducted by Martínez-De-Pisón, Pernía,

Table 1
Sections within the HDGL.

Area	Description
Pre-heating (PRE)	Strip pre-heating and cleaning area
Heating: sub-areas 1–8 (01–08)	Sub-areas 1–8 of the heating area of the furnace, where the strip temperature is raised to around 850 °C
Holding: sub-areas 9 and 10 (09–10)	Area where the strip temperature is held around 850 °C: Sub-areas 9 and 10
Slow cooling (ENL)	Area where the strip is cooled slowly to 600–650 °C
Rapid cooling (ENR)	Area where the strip is cooled rapidly to 400–450 °C
Aging (IGU)	Area where the strip temperature is equalized before being dipped into the zinc pot
Zinc pot (BATH)	Molten zinc bath dipping area
Equalizer (TRM)	Equalizer area
General (–)	Parameters which are constant throughout the HDGL

Table 2
Main groups of variables.

Name	Type	Description
CODE	Nominal	Coil code
CON_H2	Numeric	H_2 concentration in the air in area *xx*
CON_O2	Numeric	O_2 concentration in the air in area *xx*
TMP_PR	Numeric	Dew point temperature in that area
Zxx_TMP	Numeric	Temperature of area *xx*
TMP_Pxx	Numeric	Strip temperature measured with pyrometer xx in each process area
THICK, WIDTH	Numeric	Steel strip thickness and width
SPD	Numeric	Strip feed rate (m/min)
BATH_TMP	Numeric	Zinc bath temperature
CMP_BATH	Numeric	Chemical composition of zinc bath. Percentages of main chemical elements in bath
CMP_STEEL	Numeric	Chemical composition of the steel strip. Percentages of main chemical elements
ADHERENCE	Binary	Whether zinc coating adherence is within tolerances (0) or not (1)

Jiménez-Macías, and Fernández, 2010; Martínez-De-Pisón, Pernía, González, López-Ochoa, and Ordieres (2010); and Martínez-De-Pisón, Celorrio, Pérez-De-La-Parte, and Castejón (2011).

The selected variables corresponded to measurements taken in each one of the process zones (Table 1). For each one of these zones, the time series were recorded for the following: air composition (in percentage of H_2 and O_2), the temperature in each zone, the temperature of the steel strip recorded at several points and taken using pyrometers, strip velocity and dewpoint temperature in various process zones, amongst others (Table 2). In addition, inclusion was made of the dimensions of each coil (width and thickness), chemical composition of the steel in each coil processed, as well as the temperature and composition of the zinc bath. All the measurements were taken linearly every 100 m along the steel strip. Accordingly, each value for each time series corresponded to the mean of the readings taken for 100 m of steel strip.

The output variable was a binary value of "GOOD" or "BAD" that indicated whether the thickness of the zinc coating was acceptable ("GOOD") or not ("BAD").

4.4. Pre-processing and segmentation of the time series (steps: 1, 2, 3 and 4)

Following the selection of the more representative process variables, a battery of filters was selected for each time series. The filtering of each time series was designed to extract the basic form of the same in order to facilitate the subsequent process of extracting episodes.

Basically, the choice for most of the variables involved filters that screened below a threshold value in order to eliminate zeros or very low values due to data gathering failures or sensor deficiencies. Filters of this kind use the last valid value recorded at instant $t-1$ to replace zero values or those below a set threshold for instant t. In addition, inclusion was made in most cases of sliding-window filters with Gaussian functions of widths between 5 and 20 in order to smooth the final series and obtain the signal's basic shape. Figs. 2 and 3 show two examples of filtering applied to two process temperatures, respectively.

Once the basic shapes had been obtained for each one of the time series, the next step involved obtaining the most significant maxima and minima with a view to extracting the most significant episodes. In most variables, the most appropriate values of R according to (1) and (2) ranged between 1.001 and 1.009. The aim was to extract the truly significant maxima and minima for each time series.

The next step was to extract the characteristic events from each one of them. Table 3 shows the 120 types of significant events which were deemed useful for seeking knowledge according to Fig. 4.

For simplification purposes, each episode corresponded to a single event extracted from the 120 defined in Table 3. Therefore, Step 4 in the method was not taken as there was insufficient background to successfully form the complex sequences of events called episodes. In spite of this, the method is fully valid for the practical case studied.

In general, some episodes extracted correspond to moments when the time series were higher or lower than a specific value: for example when the concentrations of O_2 and H_2 were below a threshold or when the area temperature, the zinc bath temperature, the strip temperature or the strip feed rate were above or below a certain value. Other episodes are moments when variables such as the area temperature, the strip temperature or the strip feed rate fluctuated significantly (not horizontal episodes, NOT_HOR).

For the chemical compositions of the zinc bath and the type of steel in the coils, events were generated only in those cases when the mean Euclidian distance of each composition in each coil was significantly high, i.e. when the steel detected in the coils or the zinc bath composition was very different from usual.

The events in Table 3 and the values of the search parameters for each one of them were defined with the help of on-site technicians. In compliance with the confidentiality agreement reached with the company, the final values of the parameters used for extracting the events cannot be disclosed.

4.5. Creating the episode database T (Step: 5)

Once all the significant episodes or itemsets had been found for each time series analyzed, the episode database T was built, with each transaction corresponding to the itemsets that appeared at a given moment, within a time window width of 80 ut (8000 strip meters), with the consequent set to "ADHERENCE_BAD" and a time-lag of zero (Fig. 10).

Table 3
Types of episode defined.

Name	Number	Type	Description
CON_H2_Zxx_BELOW	10	BELOW	H2 concentration in the air in zone *x* below a threshold
CON_O2_Zxx_BELOW	10	BELOW	O2 concentration in the air in zone *x* below a threshold
Zxx_TMP_OVER	10	OVER	Temperature of area *xx* over a threshold
Zxx_TMP_BELOW	10	BELOW	Temperature of area *xx* below a threshold
Zxx_TMP_NOT_HOR	10	NOT_HOR	Temperature of area *xx* with big changes (not homogeneous)
TMP_Pxx_OVER	11	OVER	Strip temperature measured with pyrometer *xx* over a threshold
TMP_Pxx_INC	11	INC	Strip temperature measured with pyrometer *xx* with high increment
TMP_Pxx_DEC	11	DEC	Strip temperature measured with pyrometer *xx* with high decrement
TMP_Pxx_BELOW	11	BELOW	Strip temperature measured with pyrometer *xx* below a threshold
TMP_Pxx_NOT_HOR	11	NOT_HOR	Strip temperature measured with pyrometer *xx* with big changes (not homogeneous)
THICK_OVER	1	OVER	Steel strip thickness over a threshold
THICK_BELOW	1	BELOW	Steel strip thickness below a threshold
WIDTH_OVER	1	OVER	Steel strip width over percentile 95
WIDTH_BELOW	1	BELOW	Steel strip width below percentile 5
SPD_OVER	1	OVER	Strip feed rate over a threshold
SPD_BELOW	1	BELOW	Strip feed rate below a threshold
SPD_INC	1	INC	Strip feed rate with high increment
SPD_DEC	1	DEC	Strip feed rate with high decrement
SPD_NOT_HOR	1	NOT_HOR	Strip feed rate with big changes (not homogeneous)
BATH_TMP_OVER	1	OVER	Zinc bath temperature over a threshold
BATH_TMP_BELOW	1	BELOW	Zinc bath temperature below a threshold
BATH_TMP_NOT_HOR	1	NOT_HOR	Zinc bath temperature big changes (not homogeneous)
BATH_CMP__OVER	1	OVER	Mean of Euclidean distance of chemical composition of zinc bath to other coils over a threshold
STEEL_CMP_OVER	1	OVER	Mean of Euclidean distance of the steel. Percentages of main chemical elements: Fe, Mn, Al, Ni, etc. to other coils over a threshold
ADHERENCE_BAD	1	LABEL	Zinc coating adherence outside tolerances

In other words, whenever a failure was detected due to the poor adherence of the zinc coating (ADHERENCE_BAD), a search was made for those episodes or items recorded over the preceding 8000 m of strip. The episodes found, which had occurred just before the appearance of the poor adherence, were stored in *T*.

As the poor adherence of the zinc coating affected 39 steel coils, by the end of the process the *T* database consisted of 39 rows or lists of major episodes occurring prior to the zinc coating's adherence failure.

4.6. Searching for association rules (Step 6)

The search process for frequent itemsets or episodes for the antecedent was performed with the ECLAT algorithm and a

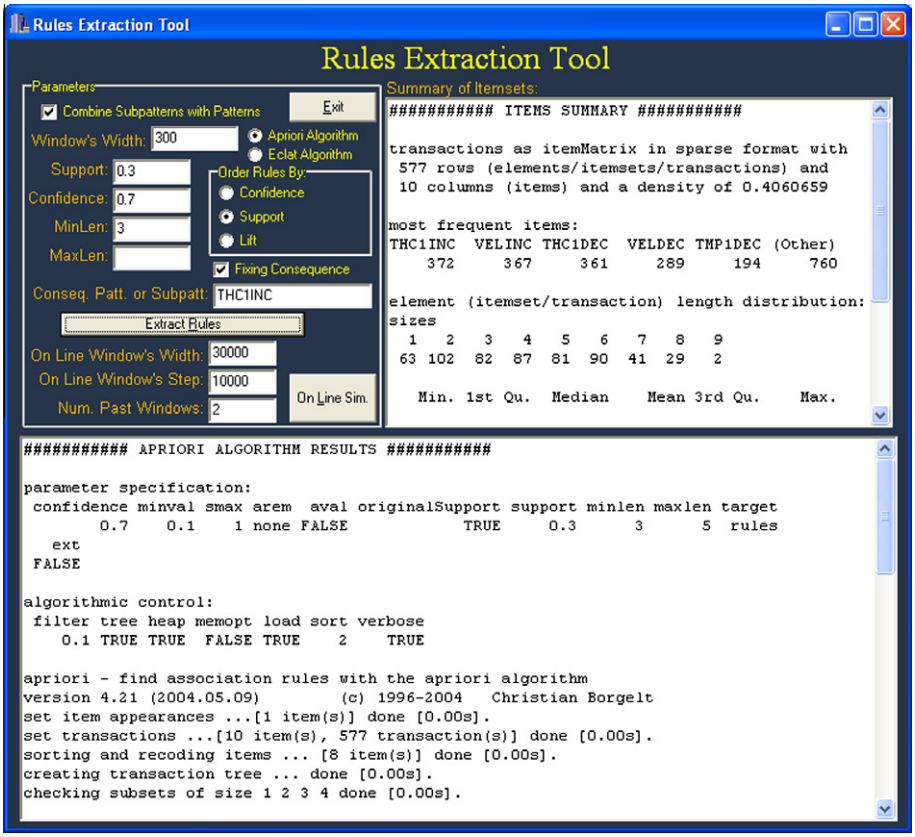


Fig. 10. Example of CONOTOOL rule extraction window.

minimum *RelSupportWinRule* of 50%. There were 64 frequent itemsets or episodes with a *RelSupportWinRule* higher than 50%. Table 4 shows the first 20 frequent itemsets ordered from larger to smaller according to the *RelSupportWinRule* and accompanied by the *RelConfidenceWinRule* for each one of the rules extracted.

The frequent itemsets or episodes obtained were analyzed visually in order to obtain useful hidden knowledge that would explain the causes of the faults recorded on the steel coils. The analysis of the results considered the values of both *RelSupportWinRule* and *RelConfidenceWinRule*, as well as the true significance of each one of the rules extracted.

Table 4
First 20 rules extracted (arranged by support). Highlighted in bold are the two interesting rules with the highest *RelConfidenceWinRule*.

Num.	Items	*RelSupportWinRule*	*RelConfidenceWinRule*
1	{Z06_TMP_BELOW}	0.77	0.53
2	{TMP_P02_BELOW}	0.69	0.45
3	**{BATH_TMP_BELOW SPD_DEC Z06_TMP_BELOW}**	**0.67**	**0.76**
4	{BATH_TMP_BELOW Z06_TMP_BELOW}	0.67	0.60
5	{BATH_TMP_BELOW SPD_DEC}	0.67	0.62
6	{SPD_DEC Z06_TMP_BELOW}	0.67	0.62
7	{Z06_TMP_BELOW TMP_P02_BELOW}	0.67	0.45
8	{SPD_DEC}	0.67	0.60
9	{BATH_TMP_BELOW}	0.67	0.72
10	{BATH_TMP_BELOW SPD_DEC Z06_TMP_BELOW TMP_P02_BELOW}	0.62	0.55
11	{BATH_TMP_BELOW SPD_DEC Z06_TMP_BELOW SPD_NOT_HOR}	0.62	0.55
12	{BATH_TMP_BELOW SPD_NOT_HOR MP_P02_BELOW TMP_P02_BELOW}	0.62	0.55
13	{BATH_TMP_BELOW Z06_TMP_BELOW SPD_NOT_HOR TMP_P02_BELOW}	0.62	0.72
14	{BATH_TMP_BELOW Z06_TMP_BELOW SPD_NOT_HOR}	0.62	0.73
15	**{BATH_TMP_BELOW SPD_NOT_HOR TMP_P02_BELOW}**	**0.62**	**0.80**
16	{BATH_TMP_BELOW SPD_DEC SPD_NOT_HOR}	0.62	0.58
17	{SPD_DEC Z06_TMP_BELOW SPD_NOT_HOR TMP_P02_BELOW}	0.62	0.55
18	{SPD_DEC Z06_TMP_BELOW SPD_NOT_HOR}	0.62	
19	{SPD_DEC SPD_NOT_HOR TMP_P02_BELOW}	0.62	0.65
20	{Z06_TMP_BELOW SPD_NOT_HOR TMP_P02_BELOW}	0.62	0.70

Table 4 shows that the majority of the frequent episodes found involve combinations of a small group of events {(Z06_TMP_BELOW), (TMP_P02_BELOW), (BATH_TMP_BELOW), (SPD_DEC, Z06_TMP_BELOW5) and (SPD_NOT_HOR)} which appear in almost all the rules and which form redundant rules, albeit with different values of *RelConfidenceWinRule*. It should be remembered that *RelConfidenceWinRule* explains the number of times the antecedent appears when the consequent occurs, in this case faulty zinc coating (ADHERENCE_BAD), divided by the number of times the antecedent appears in the entire database, although always within a window with a previously defined width, which in this case is 80 ut (equivalent to 8000 strip meters). Accordingly, a low value indicates a weak relationship between the antecedent and the consequent as the antecedent appears regardless of whether or not the consequent occurs; by contrast, a high value of *RelConfidenceWinRule* indicates a cause cause–effect relationship between the antecedent and the consequent. Highlighted in bold are the two rules (3 and 15) with the highest *RelConfidenceWinRule* and, therefore, the most interesting ones to analyze:

[3] IF {(BATH_TMP_BELOW) & (SPD_DEC) & (Z06_TMP_BELOW)}
THEN **ADHERENCE_BAD** WinW = 80, TimeLag = 0
(RelSupportWinRule = 67%,
RelConfidenceWinRule = 76%)

[15] IF {(BATH_TMP_BELOW) & (SPD_NOT_HOR) & (TMP_P02_BELOW)}
THEN **ADHERENCE_BAD** WinW = 80, TimeLag = 0
(RelSupportWinRule = 62%,
RelConfidenceWinRule = 80%)

The first knowledge rule reveals that when the temperature in the zinc bath is low (*BATH_TMP_BELOW*), the temperature in zone 6 of the furnace is also low (*Z06_TMP_BELOW*) and the strip feed rate falls sharply (*SPD_DEC*), coinciding with faulty zinc coating (*ADHERENCE_BAD*). This occurred with 67% of database *T* and the consequent was fulfilled 76% of the times when the antecedent appeared. In other words, this rule is fulfilled 67% of the times there has been an adherence fault. Furthermore, it is a rule with a high confidence level, as 76% of the times the antecedent has occurred there has also been an adherence fault.

The second knowledge rule indicates that sudden changes in velocity (*SPD_NOT_HOR*) together with low zinc bath temperatures (*BATH_TMP_BELOW*) and low strip temperatures at the furnace outlet (*TMP_P02_BELOW*) lead to errors in the zinc coating in 62% of database *T*. This was fulfilled 80% of the time. In other words, 62% of the faulted coils have been preceded by the episodes described in this rule's antecedent. In addition, 80% of the times the antecedent has occurred there have also been coating faults on the coils.

As with most instances of research into association rules, most of the other rules involved episodes similar to rules 3 and 15 but with a lower *RelConfidenceWinRule*, so they were deemed to be weaker than the former two.

Finally, other rules such as the first and second ones were not considered important as their *RelConfidenceWinRule* values were too low.

In short, the two rules extracted, with high values for *RelSupportWinRule* and *RelConfidenceWinRule*, had useful hidden knowledge for identifying the causes of adherence failure in a high percentage of defective coils. Accordingly, the identification of the rules' most characteristic episodes enabled on-site technicians to know which parts of the process should be the focus of corrective and surveillance actions in order to reduce the adherence defects affecting the zinc coating.

5. Conclusions

This paper presents an experiment based on simple pre-processing, segmentation and a search for hidden knowledge on. the basis of time series that can be easily applied to the enhancement of production processes. The pre-processing and segmentation of time series linked to the use of association rule algorithms may be extremely useful when searching for hidden knowledge in the data logs of industrial processes, which may help to improve production processes.

The experiment has shown that techniques of this nature depend heavily on the expertise of the analyst and that the "human factor" is vital at all the stages proposed in this methodology. An interesting improvement may involve using the logic of fuzzy associations in order to seek more flexible sequences akin to human thought processes. The technique has been proposed for frequent episode mining to detect the performance of network intrusion detection systems (Luo & Bridges, 2000).

On a practical level, the conclusion drawn is that by means of iterative and interactive adjustments of the pre-processing and segmentation functions (filters, detection of significant maxima and minima, definition and extraction of episodes) experts can obtain significant rules more reliably than in fully automatic rule extraction systems. We therefore consider it worthwhile to make the effort required to develop tools to facilitate iteration for experts and analysis software in all pre-processing and time series segmentation tasks.

All the pre-processing and segmentation algorithms for time series were implemented via the free statistical analysis program R (R Development Core Team, 2008) within a library called *KDSeries*. Furthermore, given the enormous effort in trial and error that is required at these stages, it was decided to develop a new visual tool called CONOTOOL to make these tasks easier. This tool allows a more intuitive, speedier use of all the functions in the *KDSeries* library. The latest available versions of both the *KDSeries* library and *CONOTOOL* can be downloaded from the CONOSER Project website: http://api.unirioja.es/conoser.

It is worth noting that tools of this kind can be used not only for extracting knowledge from industrial processes but also extrapolated, with the same degree of success, to other fields such as the environment, network systems, business, and marketing.

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Chapter 4

PUBLICATION II

Sanz-García, A., Fernández-Ceniceros, J., Fernández-Martínez, R. & Martínez-de-Pisón, F. J. (2012). Methodology based on genetic optimisation to develop overall parsimony models for predicting temperature settings on an annealing furnace, *Ironmaking & Steelmaking*, available on line. DOI 10.1179/1743281212Y.0000000094.

Methodology based on genetic optimisation to develop overall parsimony models for predicting temperature settings on annealing furnace

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Developing better prediction models is crucial for the steelmaking industry to improve the continuous hot dip galvanising line (HDGL). This paper presents a genetic based methodology whereby a wrapper based scheme is optimised to generate overall parsimony models for predicting temperature set points in a continuous annealing furnace on an HDGL. This optimisation includes a dynamic penalty function to control model complexity and an early stopping criterion during the optimisation phase. The resulting models (multilayer perceptron neural networks) were trained using a database obtained from an HDGL operating in the north of Spain. The number of neurons in the unique hidden layer, the inputs selected and the training parameters were adjusted to achieve the lowest validation and mean testing errors. Finally, a comparative evaluation is reported to highlight our proposal's range of applicability, developing models with lower prediction errors, higher generalisation capacity and less complexity than a standard method.

Keywords: Hot dip galvanising line, Annealing furnace, Genetic algorithms, Artificial intelligence, Overall models, Parsimony criterion

List of symbols

Al, Cu, Ni, Cr, Nb	chemical composition of steel, wt-%
C, Mn, Si, S, P	chemical composition of steel, wt-%
G	total number of generations
I	number of best individuals for early stopping
J	fitness function
P	population size
q	binary array for feature selection array
RMSE	root mean squared error
T	period of stability
THC1	zone 1 set point temperature (initial heating zone), °C
THC3	zone 3 set point temperature (intermediate heating zone), °C
THC5	zone 5 set point temperature (final heating zone), °C
ThickCoil	strip thickness at the annealing furnace inlet, mm
TMPP1	strip temperature at the heating zone inlet, °C
TMPP2	strip temperature at the heating zone outlet, °C
TMPP2CNG	strip set point temperature at the heating zone outlet, °C
V, Ti, B, N	chemical composition of steel, wt-%
VelMed	strip velocity inside the annealing furnace, m min^{-1}
W	complexity term
WidthCoil	strip width at the annealing furnace inlet, mm
x	user-defined fraction or proportion
δ	generation defined penalty coefficient
λ	chromosome
Λ	population array
μ	weighting coefficient of complexity term
σ	normalisation coefficient
χ	mutation factor

Subscripts

CI	confidence interval
e	elitism
g	current generation $\{1,\ldots G\}$

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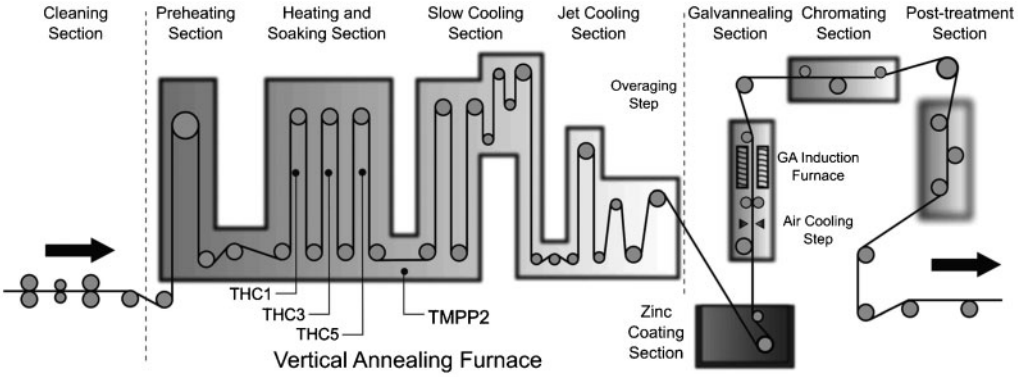


1 Basic scheme of main process in continuous HDGL

tst	testing data
val	validation data

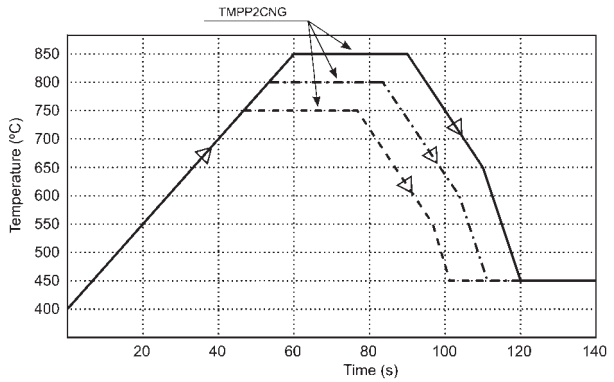
Superscripts

i	index of each individual $\{1,\ldots,P\}$
s	sorted array

Introduction

In recent times, many authors have reported that the annealing phase has a significant influence on coating steel adherence in the continuous galvanising process (Fig. 1).[1–3] When the steel strip receives a non-uniform heat treatment, it may lead to inadequate steel properties, inconsistency in the quality of the coating layer and additional coating problems, including surface oxidation and carbon contamination.[4] The standard operating mode on a continuous hot dip galvanising line (HDGL) usually involves determining the optimal settings to ensure a suitable thermal annealing treatment for each type of steel coil (Fig. 2) and a correct temperature distribution before the zinc bath. Accordingly, proper temperature adjustment inside the continuous annealing furnace (CAF) is the main task because the final temperature has to be uniform over the whole length of the strip and very close to a pre-established optimal value for the proper application of the zinc coating. However, current control systems face numerous problems when dealing with new steel coils that have not been previously mapped. The following disadvantages are generally found for most of these models.

First, their implementation in a galvanising line requires the generation of one non-linear model for almost every one of the products manufactured.



2 Three profiles of annealing treatment with two phases in cooling section

Second, model coefficients require several adjustments over time to adapt to new processing conditions. In the case of data driven models, the development is conducted offline through an iterative training process using available historical data and requiring long periods of time.

Third, models are unable to maintain the accuracy of outputs for the products that have not been previously processed. Continuous variations in coil dimensions and the chemical compositions of the steel hinder their direct implementation in a real time control system.

More research in modelling, system identification and control system design is still needed to address the problem of dealing with new steel coils that have not been previously mapped. In particular, enhancing the non-linear modelling of the CAF for predicting temperature settings is crucial on an HDGL to improve furnace temperature regulation and homogenise strip temperature. The main requirement is that the models should efficiently learn from historical data and then uphold accuracy in response to new operating conditions. To this end, resulting models need to be more parsimonious for maximising their generalisation capability. In short, even though previous research has already shown significant improvements,[5,6] developing new overall and parsimony prediction models is still an unresolved challenge for control systems in HDGL.

Related research

An alternative to the model based approach is the implementation of data driven models that take into account not only the inherent non-linearities of heat treatments but also the plant operators' know how and historical data.[7,8] Research has revealed a growing interest in artificial intelligence models in recent years.[9] For instance, neural based models have also been widely used for modelling steelmaking processes: forecasting breakouts in the continuous casting of slab,[10] supervising the control of a reheating furnace,[11] calculating the rolling force for a rolling mill process control system,[12] productivity, CO_2 content of the top gas and Si content in a blast furnace,[13] estimating sinter quality and sinter plant performance indices in a steel plant,[14] predicting mechanical properties and microstructural evolution in hot rolled steel strip,[15] etc. More particularly, in HDGL, Lu and Markward[16] reported significant improvements using artificial neural networks for coating control, Schiefer *et al.*[17] presented a combination of clustering and a radial basis function network to

improve predictions in the online control of the galvannealing process and, lastly, another approach using multilayer perceptron (MLP) was used by Pernía *et al.*[18] to estimate the velocity set point for each kind of coil.

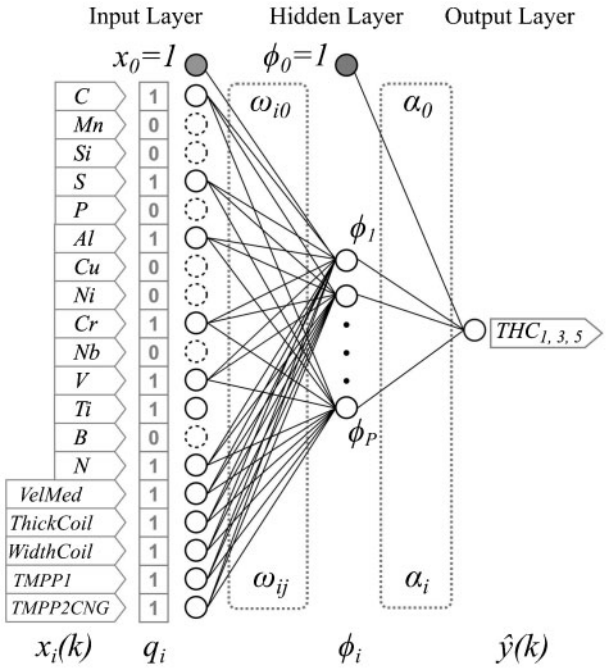
Along with this research, other promising papers have emerged to develop more reliable models for predicting CAF temperature settings in HDGL. In an early paper, the authors reported a methodology based on combining MLP neural networks and genetic algorithms (GAs).[19] The results showed that MLP can predict the optimal settings of a CAF control system. Nevertheless, the task of finding the best MLP topology is still a challenging problem. In 2010, the authors provided support for using MLPs with few hidden neurons instead of more complex networks to predict CAF temperature settings, in particular dealing with data not previously encountered.[20] Based on previous papers, in 2010, the authors proposed an overall dynamic model for the strip temperature in the annealing furnace.[20] Finally, an optimisation of the annealing cycle combining models developed in previous papers has also been reported recently by the authors.[21] This combination allowed satisfactory heat treatments even in cases of sudden changes in strip specifications, such as welding two coils that are totally different in terms of dimensions and chemical composition.

The advent of GAs, which are widely used in many industrial domains,[22] has meant that the task of finding an optimal neural based model has become more of a tractable problem. Genetic algorithms are capable of optimising model settings, striking a balance between accuracy and complexity on the one hand and resources invested in model development on the other. In 2010, Agarwal *et al.*[13] reported on work with evolutionary neural networks to estimate the expected performance of a blast furnace with periodic variations in input parameters and changes in operating conditions. Finally, in 2011, the authors reported a method based on GAs to find the optimal MLP, with the proposal then being applied to an annealing furnace.[21]

This article focuses on GA based methodology to ensure the accuracy of predicting CAF temperature settings while processing products that have not been previously mapped. The models are required to estimate three temperature set points (*THC1*, *THC3* and *THC5*) for a CAF on an HDGL for each type of coil according to the chemical composition, dimensions and velocity of the strip. Furthermore, an assessment of the model's generalisation capacity has to be made to check whether it records a low prediction error working with coils that have not been previously processed. Selecting the most significant inputs and controlling model complexity are the common techniques used for finding the best overall model. In this paper, we furthermore introduce a penalty parameter into GA optimisation to automate the entire modelling process and select the model according to a parsimony criterion.

Methodology

The proposed methodology's main goal is the development of the most parsimonious overall model that minimises the error when estimating the temperature set points of a CAF (Fig. 1). The procedure involves using GA based optimisation to find the global solution for



3 Scheme of wrapper approach including FS and MLP neural network with one hidden layer

the optimal model parameters and the set of the most significant inputs according to a parsimony criterion. Both model complexity and overfitting are controlled by including a dynamic penalty function called a complexity term into the GA fitness function. The methodology's main component is the wrapper scheme (Fig. 3), formed by the feature selection (FS) array and the MLP. The wrapper is informed by the notion that, in the presence solely of significant variables, model accuracy may be higher and complexity lower than in cases with irrelevant variables. It should be noted that key parts of the methodology do not change when it is applied to other processes.

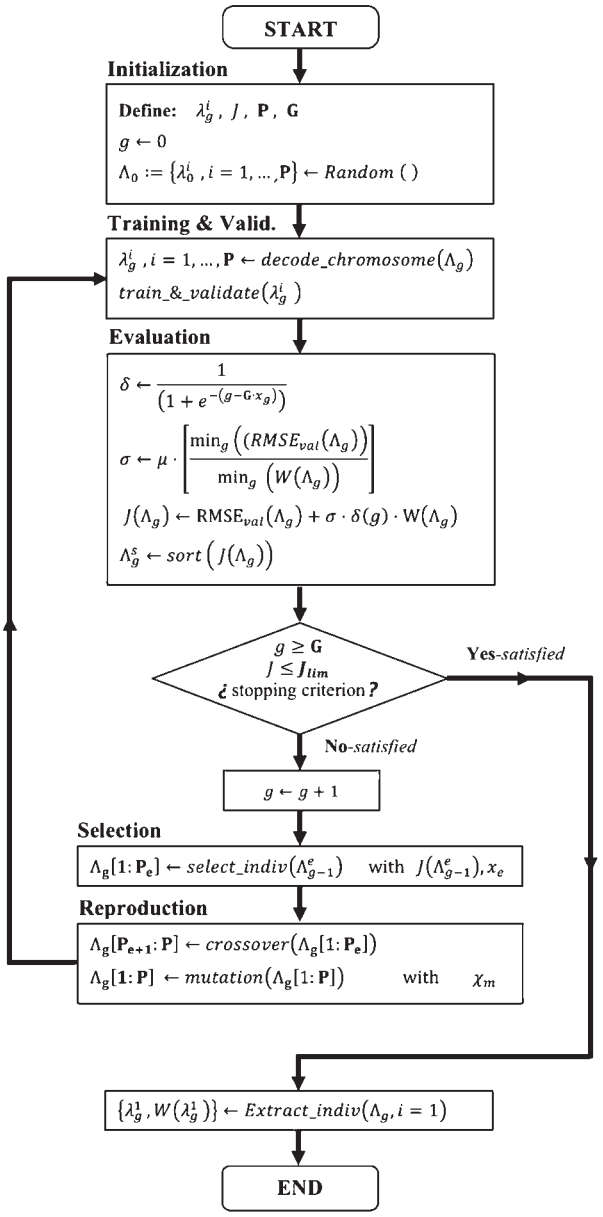
As Fig. 4 shows, the methodology begins randomly, generating the set of chromosomes λ_0^{i} of the initial population $\Lambda_0 : \{\lambda_0^1, \lambda_0^2, \ldots, \lambda_0^{\mathrm{P}}\}$. Each chromosome uses a binary format to present information about the model parameters to be optimised (*see* Fig. 5), being expressed as follows:

$$\lambda_{\mathrm{g}}^{\mathrm{i}} = [H, \eta, M, q]^{\mathrm{T}} \tag{1}$$

where H is the total number of hidden neurons, η represents the learning rate, M is the momentum and q is the binary array for FS, with 1 indicating that the input is considered and 0 indicating that it is not. Equation (2) represents the modification of the basic MLP equation that includes the FS array, i.e.

$$\hat{y}(k) = \alpha_0 + \sum_{\mathrm{i}=1}^{\mathrm{H}} \alpha_{\mathrm{i}} \phi_{\mathrm{i}} \left[\sum_{\mathrm{j}=1}^{\mathrm{L}} \omega_{\mathrm{ij}} q_{\mathrm{j}} x_{\mathrm{j}}(k) + \omega_{\mathrm{i0}} \right] \tag{2}$$

where $x_{\mathrm{j}}(k) = [x_1(k), x_2(k), \ldots, x_{\mathrm{L}}(k)]^{\mathrm{T}}$ is the input vector at instant k with length L, α_{i} and ω_{ij} are the weighting coefficients, α_0 and $\omega_{0\mathrm{j}}$ are the output and hidden layer bias respectively, ϕ_{i} is the non-linear activation function and $\hat{y}(k)$ represents the estimation of the output $y(k)$. There is no pattern in the choice of q_{i}, and the GA randomly searches through the entire range of possible feature subsets without constraints.



4 Flowchart for GA based optimisation procedure

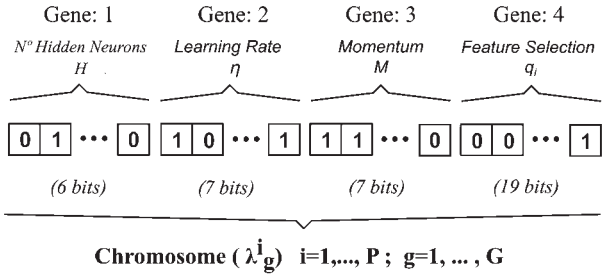
The method continues by executing the backpropagation (BP) learning algorithm for each individual of population Λ_0 to adjust MLP weights. The parameters associated to the BP learning algorithm (η and M) are also extracted from λ_0^i.

Genetic algorithm optimisation and fitness function

Adjusted models, which are parameterised by the list of α_i and ω_{ij}, are subsequently used to calculate the fitness function J. In this paper, J takes into consideration not only the criterion used for evaluating prediction errors but also a penalty function to discourage the complex models, being expressed as

$$J(\Lambda_g) = RMSE_{val}(\Lambda_g) + \delta(g)\sigma W(\Lambda_g) \quad (3)$$

where W is the complexity term calculated as the sum of squares of the weighting coefficients $\{\alpha_i, \omega_{ij}\}$, σ is a combined reduction/normalisation coefficient to make proportional W to $RMSE$ and is given by



5 Binary chromosome λ_g^i: H is integer valued, η and M are real valued, and q_i is binary coded

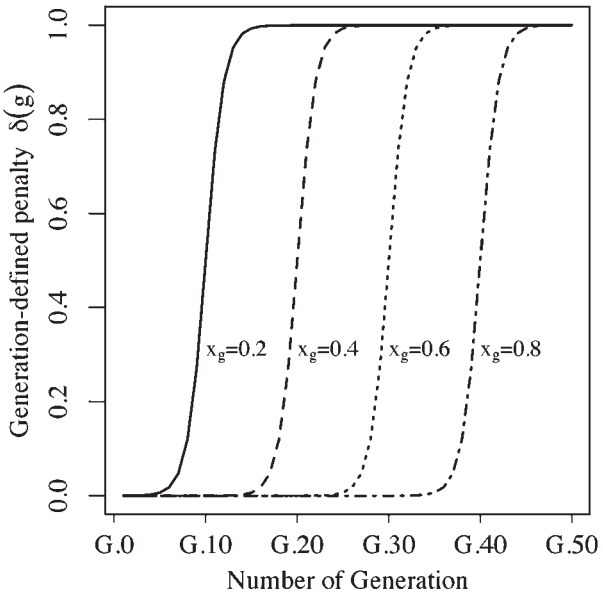
$$\sigma = \mu\{\min_g[RMSE_{val}(\Lambda_g)]/\min_g[W(\Lambda_g)]\} \quad (4)$$

where W and $RMSE_{val}$ are both the minima from current generation g, and μ is a reduction term used to weigh the relevance of the complexity term against the errors. The generation defined penalty coefficient $\delta(g)$ is included in equation (3) to represent the different impacts the weighting coefficients α_i and ω_{ij} have on the fitness function, being given as follows

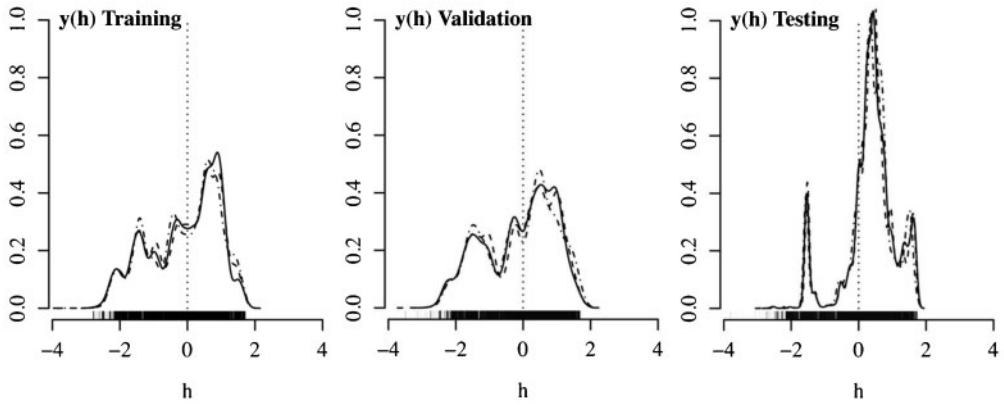
$$\delta(g) = \frac{1}{\left[1+e^{-(g-Gx_g)}\right]} \quad (5)$$

where x_g is a user defined fraction of G ranging from 0·1 to 0·9 that represents the generation where $\delta(g)$ is 50% of its final value. As Fig. 6 shows, the values of x_g affect the number of generations in which the complexity term is starting to modify the fitness function J. This time instant is crucial because the evolution of $RMSE_{val}$ makes their values lower at the beginning of the optimisation search. In sum, the less complex a model is and the more significant the selected inputs are, the lower $J(\Lambda_g)$ will be. After all the models in generation g are assigned to their associated J, the population Λ_g is sorted by increasing J values into Λ_g^e.

The evolutionary process under the principles of selection, crossover and mutation is then carried out to



6 Comparison of generation defined penalty functions $\delta(g)$ for different values of x_g



7 Density curves of training, validation and testing dataset for *THC1* (solid line), *THC3* (dashed line) and *THC5* (dotted–dashed line) temperature set points

allow chromosomes and associated models to evolve towards better solutions.

First, the best individuals $\Lambda_g[1{:}P_e]$ are selected as parents for creating the next generation Λ_{g+1} according to $J(\Lambda_g)$ and elitism percentage x_e. The rest $\Lambda_g[P_e{:}P]$ of the population g is discarded.

A crossover operator is then applied between the previously selected individuals $\Lambda_{g+1}[1{:}P_e]$ to complete the new population $\Lambda_{g+1}[P_{e+1}{:}P]$ with $(P-P_e)$ new individuals.

Finally, any new chromosomes in $\Lambda_{g+1}[1{:}P]$ may be changed through a bitwise mutation process. This genetic operator considers each gene separately and allows each bit to flip with a very low rate probability given by χ.

This is an iterative process that ends when the maximum number of generations has been reached, J is lower than a pre-established threshold or before an early stopping criterion (ESC) is satisfied. Finally, the generalisation ability of the final model is evaluated using a testing dataset consisting of new types of steel coils with a different chemical composition, width, thickness, etc. It is important to note that the optimisation process might be repeated over time to add new collected data to the initial database, with plant engineers controlling the process either automatically or manually.

Early stopping criterion for GA

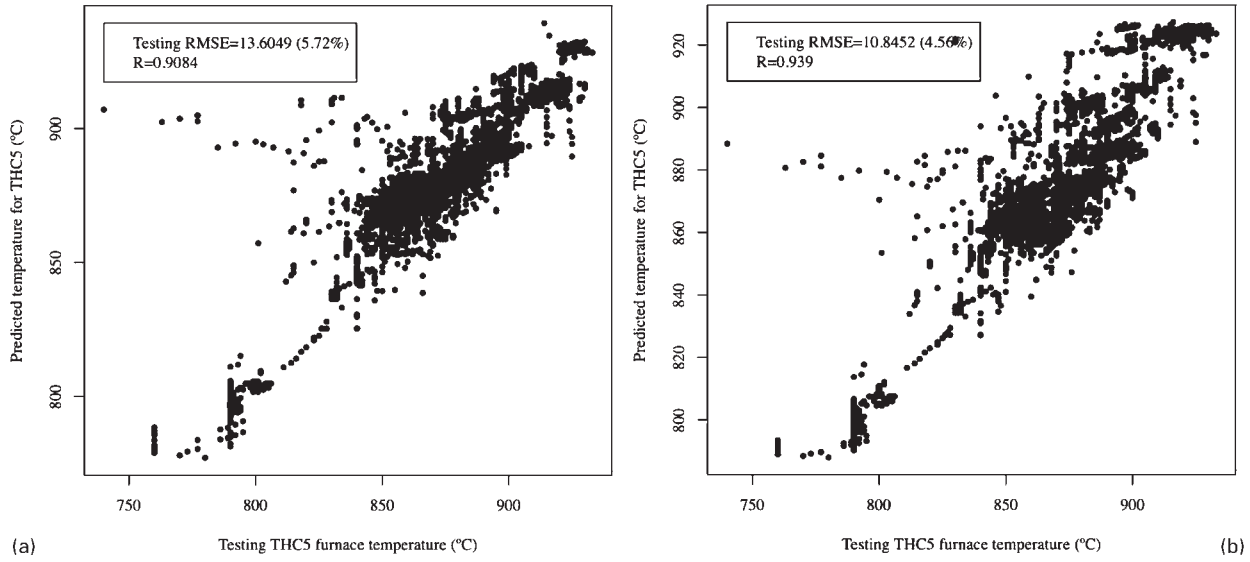
The confidence interval (CI) at a certain percentage x_{CI} represents the range of values of a variable for which the difference between the variable and its estimation is not statistically significant at a $(1-x_{CI})$ confidence level (CL). As the standard deviation S_n of a variable is a measure of its spread that is normally reported by a mean, those cases that meet the CL interval may be considered 'steady cases' in terms of the low variation in the values of the variable. Based on this approach, an ESC is proposed using $(1-x_{CI})$ values to define an interval in which the S_n of the validation model error $RMSE_{val}$ should be included to be considered a 'steady generation' for I best individuals of a generation. The number of generations forming the period of stability T is stated as the x_T percentage of the total number of generations. The criterion is based mainly on a practical procedure that searches the first subset of T generations in which I best individuals go through with having their CL lower than a low percentage x_{VAL} of the value of $[\max(RMSE_{val})-\min(RMSE_{val})]$. All threshold values should be adjusted after an initial experimental analysis of the evolution of the error $RMSE_{val}$ over several generations.

Data processing and datasets

Temperature set points and all the other variables were measured on an HDGL operating in the north of Spain. The raw database was initially formed by 56 284 observations sampled every 100 m along the strip for a total number of 2436 steel coils of different chemical compositions and under different operating conditions. In 2003, Martínez-de-Pisón preprocessed the data to improve the subsequent modelling process, and several attributes were removed after recording a high correlation with others or for not having enough metallurgical relevance in the opinion of the plant experts.[23] The preprocessed database was formed by a total number of 48 017 instances with 19 inputs and three outputs. The outputs are the furnace's three main temperature set points *THC1*, *THC3* and *THC5*. The inputs are the following attributes: *WIDTHCOIL*, *THICKCOIL*, *VELMED*, *TMPP1*, *TMPP2CNG*, *C*, *Mn*, *Si*, *S*, *P*, *Al*, *Cu*, *Ni*, *Cr*, *Nb*, *V*, *Ti*, *B* and *N*. A homogenisation process was then carried out to avoid a drastic reduction in model accuracy because the observations were extremely sparse and noisy, like most industrial databases; 721 different types of coils were identified and their positions located with 16 inputs (chemical composition, width and thickness). The same inputs were used to compute the Euclidean distance matrix for arranging the data in ascending order. The homogenised dataset was generated by sampling the same number of cases for each type of coil.

Training, validation and testing datasets

Hold out validation and k-fold cross-validation[24] are now the most widely used procedures for model selection. Both techniques can detect overfitting, but the first one is better at dealing with large databases. The authors decided to use hold out because of the size of the HDGL database, with around 49 000 observations. The sorted database was split into three non-overlapping homogeneous datasets in the following percentages: 65% training, 15% validation and 20% testing. As Fig. 7 shows, the instances were selected for inclusion in each set by stratified random sampling to



a with complexity control; *b* without complexity control

8 Predictions via measures of *THC5*

increase model reliability. The total number of instances of the training and validation datasets is 37 666, and the testing dataset was formed by 10 351 samples that will not be used during training to evaluate the generalisation ability of models.

Results and discussion

R-project was the main tool for programming, testing and monitoring experiments; especially, the R package AMORE was used to develop the prediction models.[25,26]

The search for overall parsimony models was carried out using a maximum number of generations of $G=50$ with a population size of $P=50$ individuals. Maintaining the population size at high values reduces the disadvantages of optimising real valued parameters using a binary coded GA. As Fig. 5 shows, the basic chromosome was expressed using 39 bits, and the values allowed for the chromosome parameters were as follows: $H\in\{2:50\}$, $\eta\in\{0:1\}$, $M\in\{0:1\}$ and $q_j\in\{2^0-1:2^{19}-1\}$.

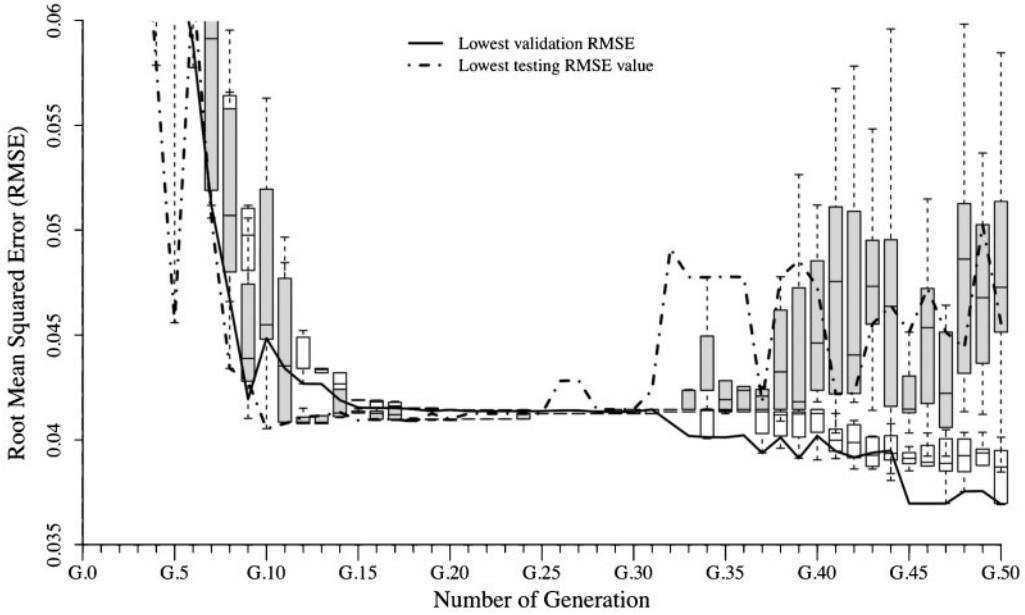
Several trials were initially conducted to adjust the GA based optimisation process, finding the following suitable values for configuration parameters: elitism percentage $x_e=20\%$, mutation factor $f_m=1{\cdot}L^{-1}=1\times39^{-1}$ and crossover proportion (one-point crossover) of 50%. The ESC was also set up in the same experiments as follows: fraction for adjusting penalty function $x_g=0{\cdot}2$, weighting coefficient of the complexity term $\mu=0{\cdot}02$, period of stability $T=10$ generations (equal to $x_T=20\%$ of $G=50$), $I=10$ best individuals per generation and percentage $x_{VAL}=0{\cdot}01\%$ for $x_{CI}=90\%$ (i.e. $x_{CL}=10\%$). The BP learning method for training MLP was also adjusted at a maximum number of 1000 epochs for an MLP composed of hidden nodes with a sigmoid activation function and an output node with a linear function.

Table 1 shows the results for the best models with validation and testing datasets for three prediction models after optimisation with and without a complexity penalty. The most important issue for finding overall models is that these should not only have a suitable prediction capability regarding the training data but also be accurate when predicting new data, such as a testing dataset. As observed, testing errors for the best models using optimisation with a complexity function did not exceed 5% *RMSE*. The number of neurons in the hidden layer and learning rate record low values, but the momentum value is significantly low. In addition to *RMSE*, Pearson's correlation coefficient *R* was also used to evaluate the linear dependence between measures and model predictions, and the proposal clearly upholds better or equal *R* values than when the complexity control is omitted (see Fig. 8).

For *THC1*, *THC3* and *THC5* prediction models, Figs. 9–11 represent, respectively, the evolution of both validation RMSE ($RMSE_{val}$) and testing RMSE ($RMSE_{tst}$) across the optimisation process with control of model complexity. Furthermore, the same processes, albeit without complexity control, are shown in

Table 1 Final results of best target models for *THC1*, *THC3* and *THC5*

	With Complexity			Without Complexity		
	THC1	*THC3*	*THC5*	*THC1*	*THC3*	*THC5*
Neurons in hidden layer	6	3	3	8	3	5
Learning rate	0·6803	0·0141	0·0050	0·0141	0·0566	0·0921
Momentum factor	0·0039	0·0039	0·0039	0·0039	0·0039	0·0039
Validation mean RMSE/%	4·13	3·22	3·71	3·81	3·23	3·33
Testing mean RMSE/%	4·12	3·33	3·29	5·09	3·31	4·54
Validation correlation	0·9842	0·9871	0·9828	0·9862	0·9872	0·9856
Test correlation	0·9714	0·9740	0·9688	0·9562	0·9734	0·9423
Stopping generation	19	26	49	21	27	49



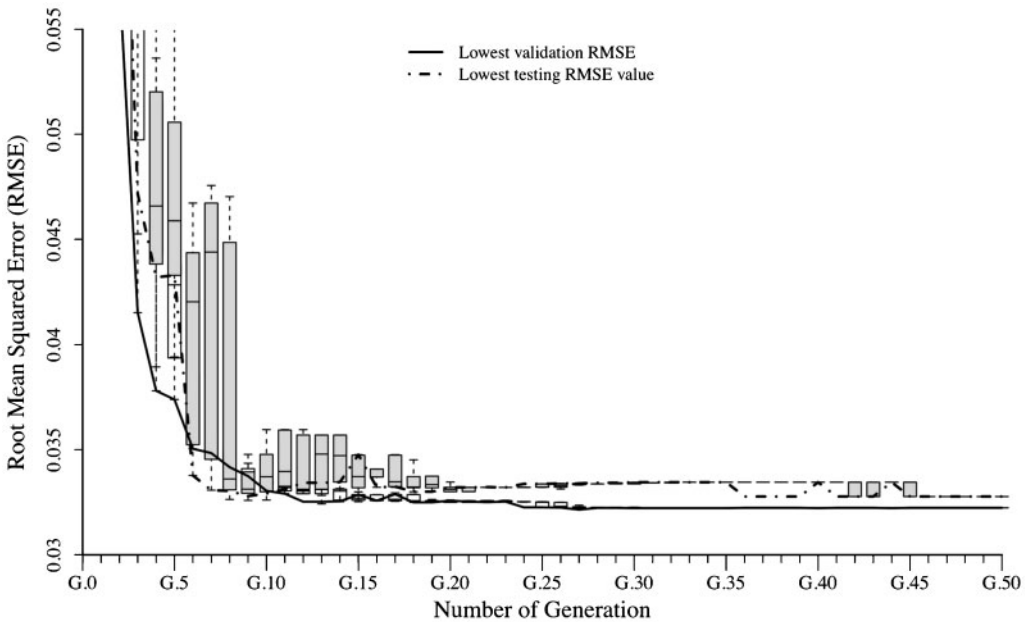
9 Evolution of $RMSE_{val}$ and $RMSE_{tst}$ (expressed as per unit values) of *THC1* models with complexity function

Figs. 12–14. It is obvious in Figs. 10, 13 and 11 that accurate models were achieved in the last generation because both $RMSE_{val}$ and $RMSE_{tst}$ are stable and of the same order of magnitude. These figures are clear illustrations of overall models, i.e. models with a low generalisation error, where $RMSE_{tst}$ is equal to or lower than $RMSE_{val}$. On the other hand, Figs. 9, 12 and 14 show three processes in which the best solution was not found in the last generation. This suggests that GA based optimisation is not automatic, and a supervisory control is necessary during the optimisation process, such as the ESC proposed.

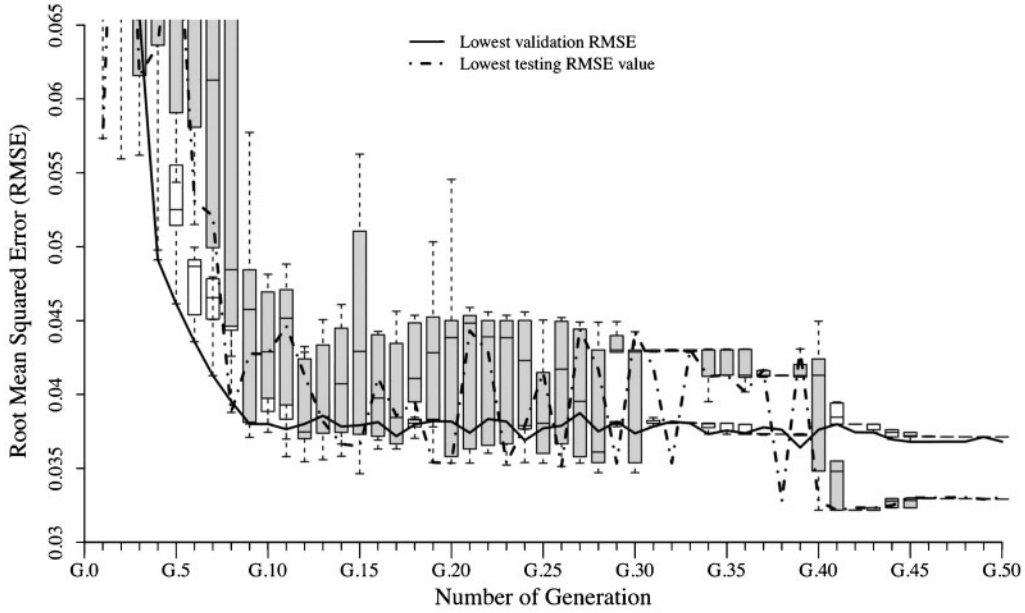
Nevertheless, even controlling evolution, Figs. 12 and 14 demonstrate that the optimisation process is unable to optimise prediction models with only the ESC. Hence, a penalty term to control model complexity was included in J, rendering it more capable of finding overall models based on the parsimony criterion. In Figs. 11 and 14, the distinction between the use and non-use of a complexity function is observed because there is no possibility of finding a subset of steady $RMSE_{val}$ values without including the complexity term in J. It is therefore true to affirm that the complexity function increased the stability of $RMSE_{val}$ and $RMSE_{tst}$, guaranteeing the existence of at least one stable period.

Figures 9–11 show that the most suitable model can be 'automatically' generated by combining the complexity control and ESC. As Fig. 9 shows, the generalisation capacity of the *THC1* model decreased from 30 to 50 generations, and the best individual in the last generation was not the best model.

These conclusions are consistent with Fig. 15. First, testing and validation errors predicting *THC1* against the complexity function W over generations are shown



10 Evolution of $RMSE_{val}$ and $RMSE_{tst}$ (expressed as per unit values) of *THC3* models with complexity function



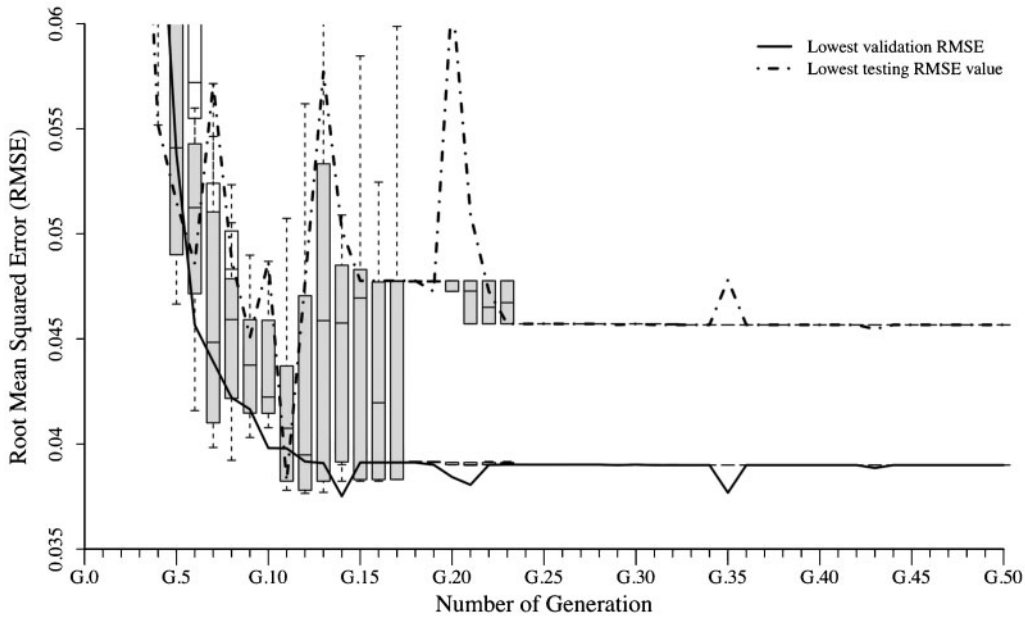
11 Evolution of $RMSE_{val}$ and $RMSE_{tst}$ (expressed as per unit values) of *THC5* models with complexity function

in Fig. 15*a* and *b* with and without complexity control, respectively. The same is applied in the case of *THC3* with Fig. 15*c* and *d* and *THC5* with Fig. 15*e* and *f*. Predicting *THC1*, the balance between $RMSE_{val}$ and $RMSE_{tst}$ is higher in Fig. 15*a* than in Fig. 15*b* because the penalty function reduced the number of overfitted models. As shown in Fig. 15*b*, the best model does not have the lowest $RMSE_{val}$, with the increase in $RMSE_{tst}$ usually being directly dependent on W. In the case of temperature *THC3*, Fig. 15*d* shows a lower density than Fig. 15*c* in the lower part of the plot, which means a sharp reduction in computational cost. Finally, Fig. 15*e* and *f* confirm that if the GA cannot find the optimal settings, the control of model complexity requires the development of less complex models (W between 5 and 8).

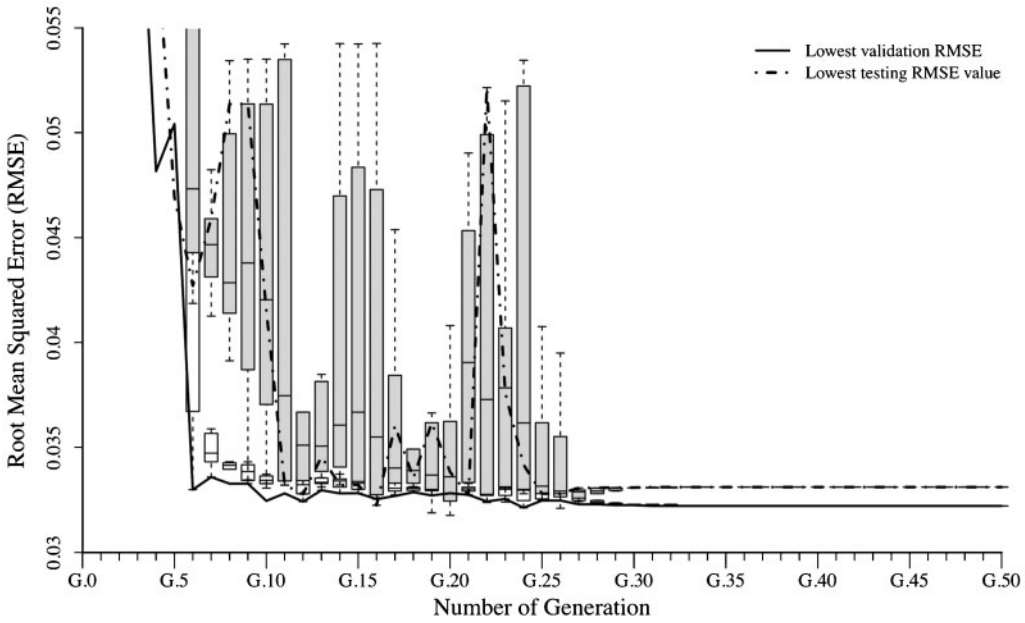
Figure 8*a* and *b* shows the predictions of the *THC5* model against the measurements for the optimisation method with and without the complexity penalty, respectively. In the case of *THC1* and *THC3*, which are not shown due to space constraints, the results were similar (see Supplementary Material) (Supplementary Material). The prediction accuracy is higher using complexity control, with absolute $RMSE_{tst}$ 10·8°C lower than $RMSE_{tst}$ and 13·6°C in the other case.

One disadvantage of GAs is the need for massive data processing. As shown in Table 1, ESC based on *CL* may reduce the total training computational cost. Using the proposed ESC,[27] we have found that the performance of the resulting models does not decrease, while the total computational costs are lower in two of the three cases studied (Figs. 9–14). Figure 9 provides support for including a stopping criterion that significantly decreases the high risk of overfitting.

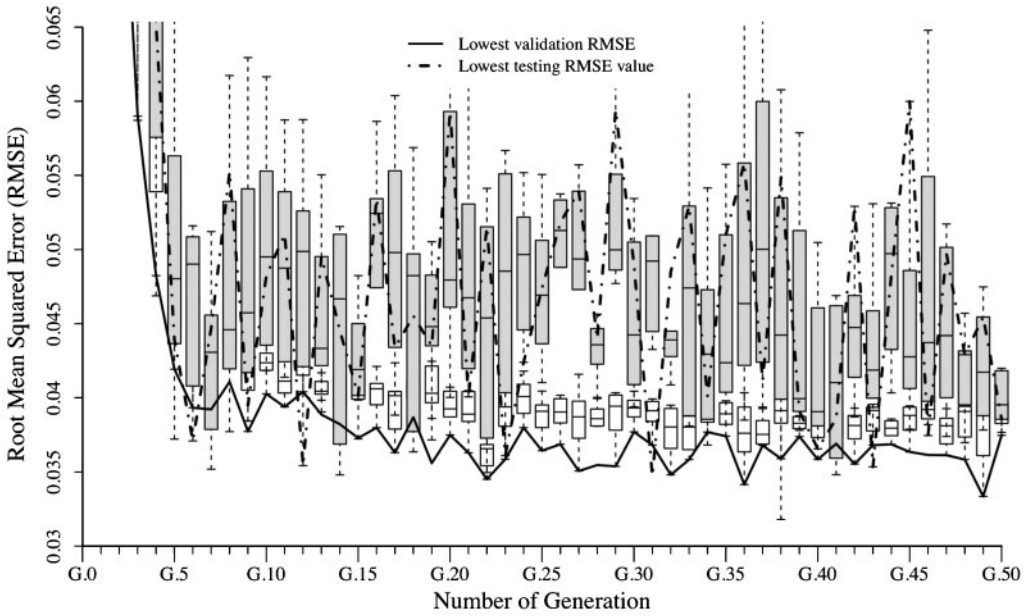
Table 2 reports the number and names of the total selected inputs by GA based FS for each final model.



12 Evolution of $RMSE_{val}$ and $RMSE_{tst}$ (expressed as per unit values) of *THC1* models without complexity function



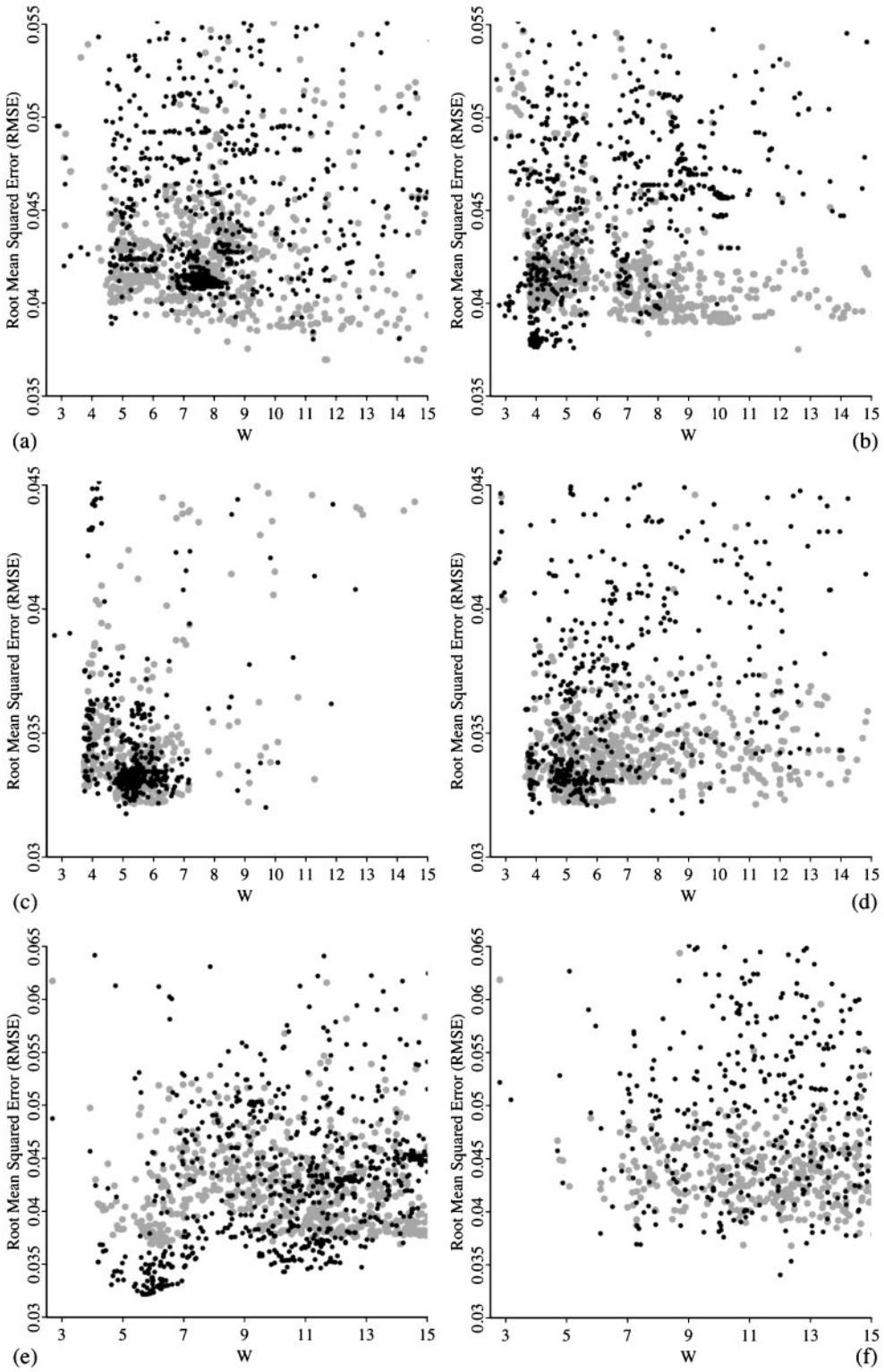
13 Evolution of $RMSE_{val}$ and $RMSE_{tst}$ (expressed as per unit values) of *THC3* models without complexity function



14 Evolution of $RMSE_{val}$ and $RMSE_{tst}$ (expressed as per unit values) of *THC5* models without complexity function

Table 2 Selected inputs of best *THC1*, *THC3* and *THC5* models: bold type indicates attributes selected in all cases, and italics in all cases except one

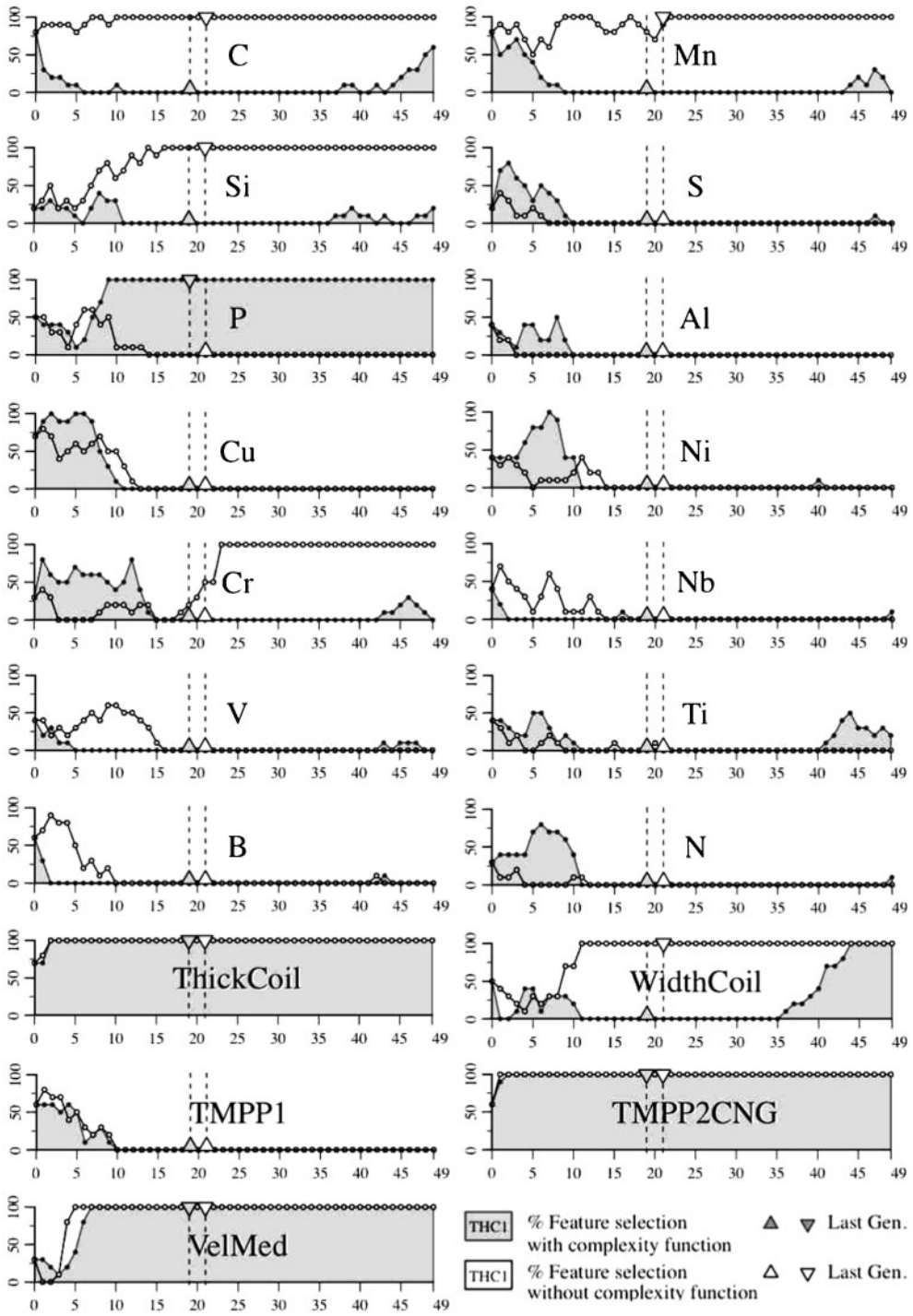
	With Complexity			Without Complexity		
	THC1	*THC3*	*THC5*	*THC1*	*THC3*	*THC5*
1	*P*	*Mn*	*Mn*	*C*	*Mn*	*Si*
2	*ThickCoil*	*Si*	*Si*	*Mn*	*Si*	*Cu*
3	*TMPP2CNG*	*S*	*P*	*Si*	*V*	*Ni*
4	*VelMed*	*ThickCoil*	*Cr*	*ThickCoil*	*N*	*B*
5	…	*WidthCoil*	*B*	*WidthCoil*	*ThickCoil*	*N*
6	…	*TMPP2CNG*	*N*	*TMPP2CNG*	*WidthCoil*	*ThickCoil*
7	…	*VelMed*	*ThickCoil*	*VelMed*	*TMPP2CNG*	*WidthCoil*
8	…	…	*WidthCoil*	…	*VelMed*	*TMPP2CNG*
9	…	…	*TMPP2CNG*	…	…	*VelMed*
10	…	…	*VelMed*	…	…	…
Total	4	7	10	7	8	9



15 Errors via aggregation coefficients *W*: *THC1 a* with complexity control and *b* without; *THC3 c* with complexity control and *d* without; *THC5 e* with complexity control and *f* without. Black points represent validation and grey points are testing data

Figure 16 complements the information on the binary selection array for *THC1* prediction models, showing the evolution of the different inputs selected for the ten best individuals over 49 generations. Stopping generation is represented using a triangle when the input was not finally selected and, conversely, an inverted triangle.

In previous research, Martínez-de-Pisón *et al.*[20] reported a substantial improvement, drastically reducing the number of variables for the chemical composition of steel using principal component analysis (PCA). However, *VelMed*, *TMPP1*, *WidthCoil*, *ThickCoil* and *TMPP2CNG* were included in the models without prior significance rating. The disadvantage of PCA is that the interpretation of the final models is more difficult as raw variables are no longer being used. In this paper, FS has been used to form a subset from all the variables without



16 Evolution of FS for 19 inputs in *THC1* models. Percentage of ten best models that include input (vertical axis) versus generation (horizontal axis)

exception to generate a parsimony model. Figure 16 plots the evolution of the selected inputs of model *THC1* for the ten best models over 50 generations; in other words, it shows each variable's significance in the accuracy of the 10 best models per generation. The figure compares the evolution of models with and without complexity control and also marks the stopping generations. In a broad perspective, some inputs like *ThickCoil*, *TMPP2CNG* and *VelMed* are significant, so maintaining these attributes as inputs enhances the accuracy of the models. This statement is consistent with previous research, where not only were these inputs selected, but also *TMPP1*. One conclusion to be drawn is that *TMPP1* is redundant and should therefore be removed as an input, as should other irrelevant attributes forthcoming from chemical components such as *Al*, *Nb* and *Ti*. Furthermore, another conclusion regarding the inclusion of a complexity term is that this makes it easier to remove irrelevant inputs, enhancing the stability of the optimisation process. For instance, the variables *Cu*, *B*, *N* and *V* reflect far less variation in models optimised with the complexity function than without.

A more specific analysis of Fig. 16 shows that the final models trained without the complexity penalty have eight inputs, and the one trained with the complexity

control has only four inputs selected, which is the same as saying we obtained half the complexity in the final models with the proposed complexity control than without. Both methods selected *VelMed*, *ThickCoil* and *TMPP2CNG*, but the method with complexity control only additionally chose attribute *P*, instead of the standard method that added *C*, *Si* and *Mn*. In this case, and according to Guyon and Elisseeff,[28] variables that are useless by themselves can be useful together. *C*, *Si* and *Mn* have the same performance together as the first model with only the variable *P*. This shows that both fitness functions have the capacity to achieve high performance models, but only our proposal generated a parsimony model. A similar behaviour was observed for *THC3* and *THC5* prediction (see Supplementary Material) (Supplementary Material).

Conclusions

This paper reports the development of a methodology based on data driven techniques for designing parsimony and overall models to predict CAF temperature set points. For plant engineers, the main advantages are the reduced complexity of the final models, better generalisation capacity and computational time saved that allow incorporating it into the CAF's online control system. The proposed methodology makes it easier for plant engineers to deal with continuous product changes, spending less time on adjusting models and reducing downtime costs.

Acknowledgements

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Chapter 5

PUBLICATION III

Sanz-García, A., Antoñanzas-Torres, A., Fernández-Ceniceros, J. & Martínez-de-Pisón, F. J. (2012). Overall models based on ensemble methods for predicting continuous annealing furnace temperature settings, *Ironmaking & Steelmaking*, available on line. DOI 10.1179/1743281213Y.0000000104.

Overall models based on ensemble methods for predicting continuous annealing furnace temperature settings

A. Sanz-Garcia, F. Antoñanzas-Torres, J. Fernández-Ceniceros and F. J. Martínez-de-Pisón*

The prediction of the set points for continuous annealing furnaces on hot dip galvanising lines is essential if high product quality is to be maintained and energy consumption and related emissions into the atmosphere are to be reduced. Owing to the global and evolving nature of the galvanising industry, plant engineers are currently demanding better overall prediction models that maintain accuracy while working with continual changes in the production cycle. This paper presents three promising prediction models based on ensemble methods (additive regression, bagging and dagging) and compares them with models based on artificial intelligence to highlight how good ensembles are at creating overall models with lower generalisation errors. The models are trained using coil properties, chemical compositions of the steel and historical data from a galvanising process operating in Spain. The results show that the potential benefits from such ensemble models, once configured properly, include high performance in terms of both prediction and generalisation capacity, as well as reliability in prediction and a significant reduction in the difficulty of setting up the model.

Keywords: Hot dip galvanising line, Continuous annealing furnace, Data mining, Process modelling, Ensemble methods, Artificial intelligence

List of symbols

Al, Cu, Ni, Cr, Nb	chemical composition of steel, wt-%
C, Mn, Si, S, P	chemical composition of steel, wt-%
N	total number of simulations or trained models
t	computation cost for training a set of models, s
THC1	zone 1 set point temperature (initial heating zone), °C
THC3	zone 3 set point temperature (intermediate heating zone), °C
THC5	zone 5 set point temperature (final heating zone), °C
ThickCoil	strip thickness at the annealing furnace inlet, mm
TMPP1	strip temperature at the heating zone inlet, °C
TMPP2	strip temperature at the heating zone outlet, °C
TMPP2CNG	strip set point temperature at the heating zone outlet, °C
WidthCoil	strip width at the annealing furnace inlet, mm
V, Ti, B, N	chemical composition of steel, wt-%
VelMed	strip velocity inside the annealing furnace, m min^{-1}
X	percentage of training data

Subscript

TH	maximum/minimum threshold value
tr	training dataset
tst	testing dataset
val	validation dataset

Superscript

ME	mean
SD	standard deviation

Introduction

The production of galvanised flat steel products has been increased over the last two decades to meet an increase in global demand, leading the galvanising industry to become a key sector in the fabric of European industry.[1] This growth has increased investments by galvanising companies with a view to increasing not only the production capacity of their continuous hot dip galvanising lines (HDGLs) but also the operational flexibility of their production plants. In fact, the search for greater flexibility is currently

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considered crucial in meeting the wide variety of customer needs, especially given today's rapidly evolving markets such as vehicle manufacturing.[2] The strategy is clear: the more different products are supplied, the more new markets will be open up. However, this required flexibility may also generate significant problems such as idle times in the continuous mode of operation or reduction in the quality of coatings. Therefore, HDGL plant engineers need to make multiple adjustments when dealing with new products until the right adherence and uniformity in coating are achieved. Reducing the time needed to determine optimal set points is also crucial for saving costs.[3]

This paper focuses on enhancing the accuracy and efficiency with which the operating set points are calculated for a continuous annealing furnace (CAF) on an HDGL. Over the last few decades, many mathematical models based on heat and mass balance have been developed to predict furnace temperature settings.[4] However, those models have some disadvantages such as clear difficulties in tuning model parameters to new product specifications, strong dependence on the experience of the engineer and long computation time to modify models. Recent papers have proved that data driven models based on artificial intelligence (AI) are a good alternative for developing accurate prediction models in the steel industry.[5] To take advantage of these techniques in the modelling of the galvanising process, the main requirements are the availability of historical data, detailed knowledge of the chemical composition of steel and time to train the models.

We propose the use of models based on ensemble methods (EMs) with high overall performance in predicting system set points.[6] The major problem of the aforementioned AI based models is that they do not maintain consistent prediction accuracy with all types of products, especially with products not previously processed. Unlike single AI based models, EMs are built using a set of models and the final output is a combination of the outputs of each individual model.[7] Ensemble methods (EMs) have the same requirements as single models, but two independent studies have shown that combining outputs from multiple predictors increase their generalisation capacity.[8,9] This may make EMs very attractive for working in rapidly changing environments.[10]

In this paper, three EMs, i.e. additive regression[11] (AR), bootstrap aggregating[6] (bagging) and dagging,[12] are developed to adjust CAF temperature settings in an HDGL. Additionally, five data driven models, i.e. least median squared linear regression[13] (LMSQ), linear regression[14] (LR), Quinlan's improved M5 algorithm[15] (M5P), multilayer perceptron neural network[16] (MLP) and support vector machine[17] (SVM), are chosen from literature as basic components of the ensembles. A comparative evaluation procedure is also included to help plant engineers select the best performing model. The results for furnace temperature set point predictions obtained with this method highlight the benefits of using EMs rather than other data driven models for the development of better overall models. Primarily, their higher generalisation capacity reduces the need for continual tuning of model parameters when dealing with new products. The additional ease with which models can be set up is the other crucial advantage for engineers.

In short, EMs have the capacity to provide high performance prediction models for online furnace control systems, leading to very low levels of divergence between the ideal annealing profile and the strip temperature actually measured.

Description of problem

A continuous HDGL is a well known industrial process composed of several independent sections, each one involving a specific treatment.[18] The heart of the annealing treatment is the CAF, which is divided up as follows: preheating area, heating and holding area, slow cooling area, jet cooling area and overaging area. Inside the CAF, the strip is recrystallised by heating it up and holding it at temperatures of between 750 and 850°C; then, the strip is cooled down at different rates to the liquid zinc bath temperature of between 450 and 470°C. In practice, full adjustment to the annealing profile prescribed can be only guaranteed by feeding the strip into the CAF at a constant speed.[19] For that reason, the control of CAF temperature settings is crucial for proper heating along the steel strip and consequently, has significant influence on the mechanical properties of the steel and the quality of the coating adherence.[20–23]

In this study, the CAF's online control system includes models for estimating three furnace temperature set points. These predictions represent a complex task, mainly due to continuous variations in product specifications and in the chemical composition of the steel used. The current data based models tend to specialise in specific groups of coils and do not maintain their accuracy with products not previously processed.[24,25] Several different models therefore need to be developed and tested to solve this problem, but this task may take up enormous amounts of time and effort. The challenge still lies in developing better overall prediction models capable of working out CAF temperature settings for new coils and different operating conditions while maintaining accuracy with no additional model training phases.

Related research

The prediction of CAF temperature settings is an unresolved challenge for enhancing the online control of the annealing process.[1] Classical approaches determine temperatures empirically on the basis of a number of process trials that generate prediction models using a set of tables.[26] This method is not efficient because there are high costs associated with in plant trials. The most widely used alternative is to develop mathematical models that consider both thermodynamic properties and heat transfer mechanics inside the CAF.[17,27–31] However, as Prieto *et al.*[32] claim, some furnace characteristics and material properties may change appreciably with different compositions and heat treatment of steel, and this may influence these models significantly. This happens, for instance, with the specific heat capacity of the strip and heating power of burners. So more than just metallurgical knowledge is required to determine precise CAF settings for each coil.[23] Developing models that are based on data may improve prediction capacity because they take into account not only the inherent non-linearities of the annealing process but also the knowhow of plant operators and historical

data.[33,34] Since 1998, several authors have reported on studies related to regression models that use historical data from steel processes.[20,35] In recent years, interest in such models has grown, especially in those based on artificial neural networks (ANNs),[2] genetic algorithm guided neural network (GA-NN) ensemble models,[36] fuzzy logic models,[37] fuzzy ANNs,[38] Bayesian models[39] and Gaussian mixture models.[40] For instance, several applications have been developed applying fuzzy set theory in HDGL for system control and quality management. Kuru and Kuru proposed a new galvannealing control system based on a fuzzy inference system that contributed to a significant improvement in the uniformity and quality of the coating layer running at lower limit of permissible coating values.[41] Recently, Zhang *et al.* proposed a feedforward control method based on fuzzy adaptive model for the thickness control process of galvanising coating.[42]

Likewise, ANNs have been successfully applied in many parts of the galvanising process. Schiefer *et al.*[43] report a combination of clustering and RBFN to improve the predictor of an online galvannealing process control. Lu and Markward[44] reduce the coating weight transitional footage by integrating ANN with the coating weight control system in an HDGL. A 2005 paper by Pernía-Espinoza *et al.*[45] shows the high performance of robust MLP estimating the velocity set point of coils inside the CAF using only their characteristics and furnace temperatures. Conversely, Martínez-de-Pisón *et al.*[46] develop similar MLPs to predict CAF temperature set points but without varying strip velocity.

Finally, the problem of finding optimal ANNs has become more tractable with the advent of genetic algorithms,[47] since which time several models have been reported with better balances between accuracy and complexity in predicting the optimal settings of the annealing process in an HDGL[48] and estimating the strip temperature during the annealing treatment inside the CAF.[49]

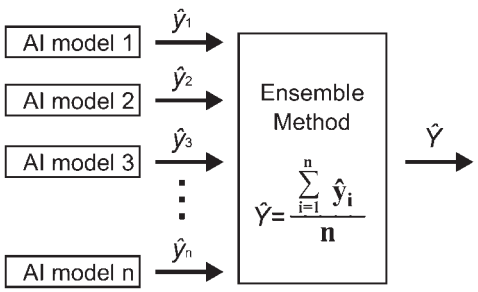
Lastly, Köksal *et al.* and Liao *et al.* presented a complete revision of most relevant data mining techniques developed during the past decade and their applications in steel and manufacturing industry.[50,51]

Methodology

Many techniques for handling regression tasks have been proposed in literature, but even today, designing automatic methodologies that choose the best performing model for a particular application remains a challenge. One current proposal is based on selecting not only the most accurate model for predicting with stored data but also the model with the highest generalisation capacity. In the following section, the methodology proposed is described on the basis of a comparative evaluation to search for the models with the best balance between accuracy, generalisation capacity and computation cost during the training phase.

Overview of models

Ensemble learning is a paradigm of ML where multiple single models, referred to as base learners (BLs), are fitted and combined to give a better solution to a particular problem. An EM constructs a set of predictors and then combines their outputs to obtain an improved single response (*see* Fig. 1). Specifically, the final output of an EM is the average or weighted average in regression tasks. Two main conditions need to be addressed for improved results to be achieved: high accuracy in all individual models and diversity between their predictions. A brief description of the EMs selected follows:



1 Basic layout of EMs by averaging a set of numerical inputs

(i) additive regression (AR) is a metamodel that enhances the performance of a regression base model. Each iteration fits a model to the residuals left by the predictor on the previous iteration. The output is obtained by adding together the predictions of all the models. The main parameter is the shrinkage or learning rate, which helps prevent overfitting and has a smoothing effect but increases the learning time[11]

(ii) bootstrap aggregating (bagging) is a metamodel that averages a number of BLs fitted with a set of different training datasets. These datasets are generated by sampling uniformly and with replacement of the original data (bootstrapping)[6]

(iii) dagging is a technique similar to bagging but in which the training datasets are created using disjoint samples. A number of disjoint, stratified folds out of the data are generated to train a BL with each subset. Dagging is potentially very suitable for BLs that are quadratic (or even worse in terms of time consumption) regarding the lowest number of instances in each training dataset.[12]

The best performing BLs then need to be selected on the basis of the support provided by previous studies.[52] Five algorithms are finally selected here from an initial list of seven, as follows:

(i) least median squared linear regression is a robust linear regression model based on classical least squares regression that minimises the median of the squared residuals. Its major disadvantage is its lack of efficiency because of its slow convergence rate[13]

(ii) linear regression is an improved version of a traditional scheme for linear predictions that includes the Akaike criterion[53] for feature selection and can also deal with weighted instances[14]

(iii) M5P tree (M5P) is an improvement of the original Quinlan's M5 algorithm for regression tasks by generating a decision tree with simple LR models at its leaves[15,54]

(iv) multilayer perceptron neural network (MLP) is a feedforward ANN that uses a supervised learning algorithm called 'back propagation' to adjust the network weights. The criterion selected for measuring the goodness of fit is usually the least mean square (LMS) error.[16] In regression, one hidden layer is usually considered due to the fact that any continuous function can be approximated with only one hidden layer if the number of connection weights is high enough[55]

(v) support vector machine is a technique with the ability to model nonlinearities resulting in complex mathematical equations. Support vector machine separates the input data, which are presented as two sets of vectors in an n dimensional space, by generating a hyperplane in the same space that maximises the margin between the two input sets.[56]

Other prediction models such as simple LR (SLR), k nearest neighbour (k-NN) and radial basis forward network (RBFN) were excluded because they previously showed lower accuracy and generalisation capacity regarding the prediction of new cases than the selected models.[46,49,52]

Evaluation and performance criteria

The most widely employed procedures for evaluating model accuracy and overfitting are hold out validation and k fold cross-validation.[57] In this paper, the former is selected because it deals better with large DBs from industrial processes. The method consists of dividing data into two non-overlapped datasets by stratified random sampling with a division ratio at percentage χ_{tr} and $\chi_{val}=1-\chi_{tr}$ for training and validation datasets respectively. The division is repeated N times, and the final errors are determined by average, increasing the robustness of the results against skewed data.

The absolute error criteria considered here are root mean squared error (RMSE) and mean absolute error (MAR). The former is expressed as

$$\mathrm{RMSE}=\left\{\frac{\sum_{k=1}^{n}\left[y(k)-\hat{y}(k)\right]^2}{n}\right\}^{1/2} \quad (1)$$

where $y(k)$ is the target output, $\hat{y}(k)$ is the prediction of the model and n is the total number of instances; the latter is defined as

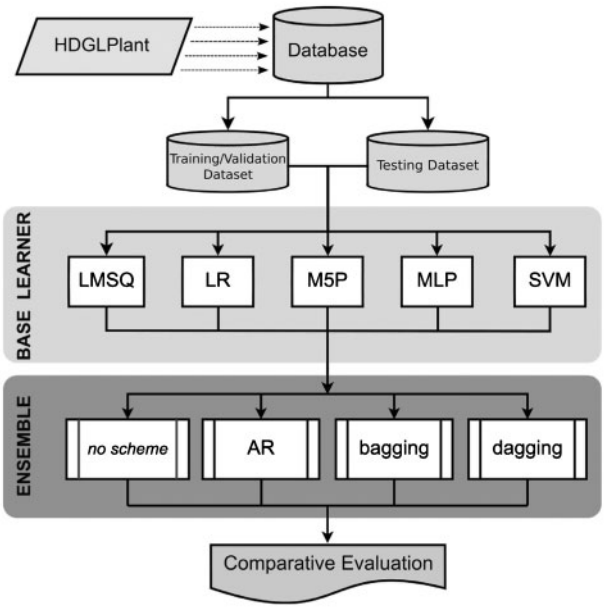
$$\mathrm{MAE}=\frac{\sum_{k=1}^{n}\left|y(k)-\hat{y}(k)\right|}{n} \quad (2)$$

From our knowledge, absolute measures are more important for comparison because they enable the actual application of models to be evaluated directly. The percentage error is also available because the data are normalised. Another performance measure is the coefficient of variation (CV), which compares the amount of variance between sets with different means and is defined as follows

$$\mathrm{CV(RMSE)}=\mathrm{RMSE^{SD}}\left(\mathrm{RMSE^{ME}}\right)^{-1} \quad (3)$$

which represents a comparative measure of the model's stability.

Finally, it is necessary to select those models that show not only good prediction capacity on modelling data but also low generalisation errors. To that end, a testing dataset with coils not included in the modelling dataset is used to check the overall capacity of models.



2 Conceptual scheme of methodology

Description of framework of experiment

The proposed framework involves the complete methodology for finding the best overall model from a set of preselected models. This prior selection is carried out using different setting parameters with each specific model and then selecting the most accurate. Figure 2 summarises the method, which is mainly divided into the following steps:

(i) creation of the DB using the data collected and subsequent division into the modelling and testing datasets by stratified random sampling. This technique homogenises the number of different cases in each dataset

(ii) developing all possible EMs combining every BL and ensemble scheme chosen with a list of preestablished parameters with no prior knowledge of performance. This is an iterative process and the values of the parameters are established according to recommendations by other authors, previous experiences or a series of initial experiments

(iii) checking of models using the testing dataset, which includes new types of steel coils and enables the generalisation error of the model to be assessed

(iv) ranking of models by a comparative evaluation to select the most appropriate for a particular application, in four steps:

Step 1: accuracy in predicting known values is evaluated by calculating the $\mathrm{RMSE_{val}^{ME}}$ of M models. Those EMs that show an $\mathrm{RMSE_{val}^{ME}} \le \mathrm{RMSE_{val}^{TH}}$, where $\mathrm{RMSE_{val}^{TH}}$ is a user defined threshold, are the only ones chosen for the next step.

Step 2: the computation cost of training M models (t) is measured to discard those EMs that take too long, i.e. $t<t^{TH}$, where the value t^{TH} is a threshold directly proportional to the complexity and size of the modelling dataset.

Step 3: a high generalisation capacity is also necessary to maintain accuracy when

models face unseen data. This is evaluated comparing the $(\mathrm{RMSE}^{\mathrm{ME}} \pm \mathrm{LSD})_{\mathrm{val}}$ and $(\mathrm{RMSE}^{\mathrm{ME}} \pm \mathrm{LSD})_{\mathrm{tst}}$, where LSD represents the least significant difference for independent values. The first value should be at least equal to the second but never much lower if the behaviour of the model is to be considered as satisfactory in terms of generalisation capacity.

Step 4: finally, the stability of the EMs is evaluated by comparing two terms: $\mathrm{RMSE}^{\mathrm{SD}}_{\mathrm{tst}}$ and the ratio $\mathrm{CV}_{\mathrm{tst}}$ for a total number of M models. Stable EMs are able to keep low variability in output errors and show very low CV when the input data are changing constantly.

In this paper, the case under study is the prediction of CAF temperature settings in an HDGL, but the method can be applied in other processes.

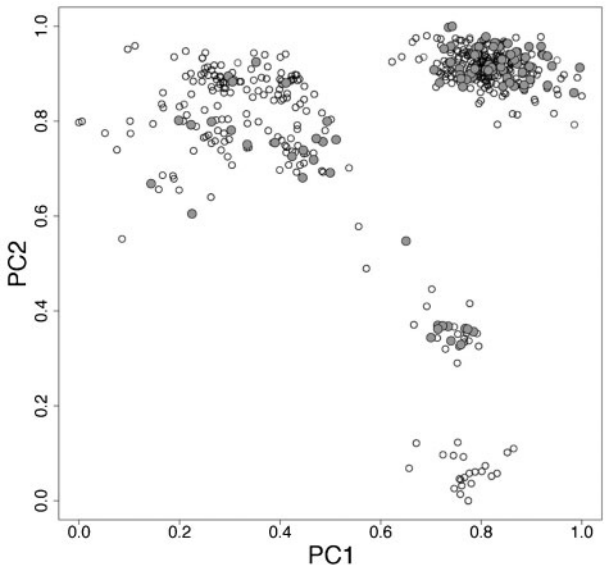
Hot dip galvanising line database for experiment

The three furnace temperature set points and other attributes were measured on an HDGL operating in Spain. The raw dataset was formed by 56 284 observations of 2436 types of coil, sampled every 100 m along the strip under different processing conditions and chemical compositions. In 2003, Martínez-de-Pisón preprocessed the raw data filtering for wrong records, detecting outliers and removing redundant variables.[26] Later, a principal component analysis[58] (PCA) was carried out to reduce the number of inputs related to the chemical composition of steel (C, Mn, Si, S, P, Al, Cu, Ni, Cr, Nb, V, Ti, B and N) to only the first seven principal axes (from PC1 to PC7), which are independent to one another and cover 87·44% of the original variance.[52] This technique appears as a black box to plant engineers and undermines the physical relationships within the chemical composition and the annealing process. Nevertheless, PCA was mainly motivated by its proved reliability, reducing the amount of data from industrial process datasets since the data used to be redundant and the variables are usually correlated.

The modelling dataset was finally formed by 49 000 instances from sampling original data until the number of coil types was homogenised. The set of inputs comprise 12 attributes (WidthCoil, ThickCoil, VelMed, TMPP1, TMPP2CNG, PC1, PC2, PC3, PC4, PC5, PC6 and PC7), and the outputs are the CAF's three temperature set points (THC1, THC3 and THC5). In the case of the test dataset, this was acquired several weeks after the data for the modelling dataset were gathered. As Table 1 shows, the test dataset is formed by 5000 instances containing 59 different types of coil but only 25 different types of steel. Finally, both datasets were normalised. Using the same datasets in this paper as in previous studies enables us to compare past models with our new proposal.[52]

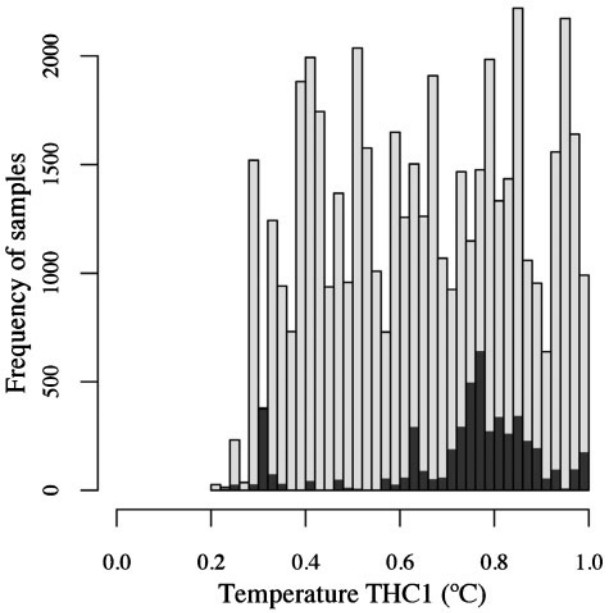
Table 1 Testing DB used to test generalisation and flexibility of models

Description	Values
Number of coils in DB	59
Different types of steels in DB	25
ThickCoil (range)	0·601–0·775 mm
WidthCoil (range)	805–1180 mm



3 Principal component analysis projection of HDGL dataset using first two principal components: circles indicate modelling data, and grey dots indicate testing data

It is advisable to take a final overview of the data before the results are explained, because the accuracy of data driven models is directly dependent on the problem that needs to be solved. Figures 3 and 4 show the modelling and testing data distributions using the first two principal axes (PC1 and PC2) and the histogram of THC1 respectively. Figure 3 reveals the existence of a large group of similar coils and several other small groups. The testing data also look evenly distributed enough over the whole range of modelling data but are extremely sparse, like most industrial data (Fig. 4). These data features decrease the prediction capacities of data driven models,



4 Histogram of attribute temperature *THC1*: light grey bars indicate modelling samples, and dark grey ones indicate testing data

Table 2 Parameter specifications for BLs

Algorithm	Parameter	Values
LR	Ridge	0·1, 0·3, …, 4
	Attribute selection	Greedy
LSMQ	Sample size	4, 8, …, 400
M5P	Min. instances/leaf	2, 4, …, 80
	Prune	True
	Unsmoothed model	False
MLP	Learning rate	0·1, 0·2, …, 0·8
	Momentum	0·1, 0·2, …, 0·6
	Num. iterations	50 000–10 000
	Num. hidden neurons	3, 5, 7, …, 40
	Decay learning rate	True
	Autoreset network	True
	Validation set size	20%
	Validation threshold	15, 25, …, 55
SVM	*C*	1·0
	E	1·0E−12
	ε parameter	0·001
	Tolerance	0·001
	Kernel type	Polynomial
	Poly. exponent	1, 1·02, …, 2·50

Table 3 Parameter specifications for ensemble schemes

Scheme	Parameter	Values
AR	Shrinkage	0·2, 0·3, …, 1
	Num. iterations	10, 20, …, 80
Bagging	Subset size	10, 20, …, 100
	Num. learning rounds	15, 20, …, 80
Dagging	Num. folds	2, 3, …, 15

but the article shows that our proposed EMs are a better way of dealing with these problems than single models.

Results and discussion

In this paper, we mainly analyse three types of EM to predict the temperature set points (THC1, THC3 and THC5) for a CAF on an HDGL. However, the results concerning THC1 are only reported to summarise the information, due to the fact that the results from training the THC3 and THC5 prediction models are similar to the first one.

The performance of models predicting THC1 is evaluated following the steps and criteria of the proposed methodology. These evaluations are carried out with the statistical software R-project 2·11[59] running on a dual quadcore Opteron server with Linux SUSE 11·2. Additionally, the models are implemented using the WEKA workbench[60] and R-project packages AMORE[61] and RWeka.[62]

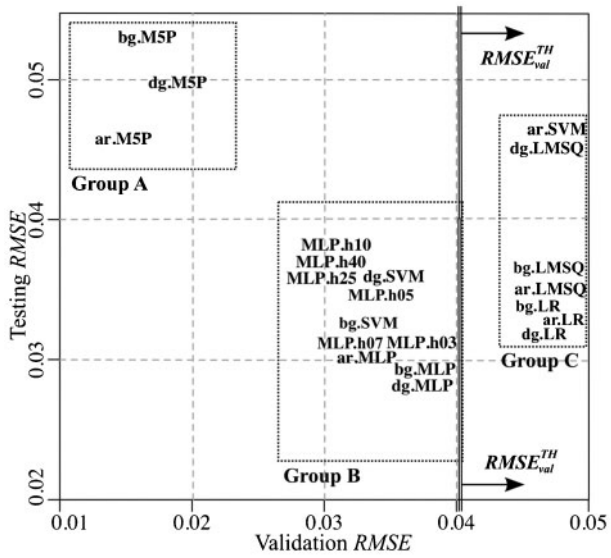
The ranges of the values of the setting parameters used to generate models with different configurations are listed in Table 2 for BLs and Table 3 for EMs. Validation and testing simulations were repeated $N=10$ times for each particular configuration, selecting only the best case for each algorithm. Table 4 presents the mean and standard deviation of both error measures (RMSE and MAE) for the best models and also the total computation time to set up a number of $M=10$ models with the same setting parameters. Likewise, Table 5 shows the results reported by Martínez-de-Pisón *et al.*[52] from earlier research into MLP models. These results allow us to discuss the advantages and disadvantages by comparing the two

Table 4 Results of modelling process for THC1 prediction models (sorted by $\mathrm{RMSE}_{\mathrm{val}}^{\mathrm{ME}}$)

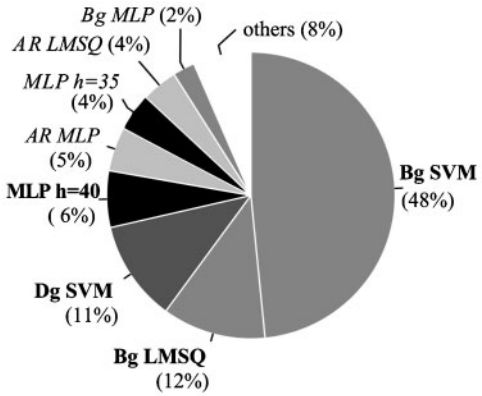
	Training error				Validation error				
Algorithm	$\mathrm{RMSE}_{\mathrm{tr}}^{\mathrm{ME}}$	$\mathrm{RMSE}_{\mathrm{tr}}^{\mathrm{SD}}$	$\mathrm{MAE}_{\mathrm{tr}}^{\mathrm{ME}}$	$\mathrm{MAE}_{\mathrm{tr}}^{\mathrm{SD}}$	$\mathrm{RMSE}_{\mathrm{val}}^{\mathrm{ME}}$	$\mathrm{RMSE}_{\mathrm{val}}^{\mathrm{SD}}$	$\mathrm{MAE}_{\mathrm{val}}^{\mathrm{ME}}$	$\mathrm{MAE}_{\mathrm{val}}^{\mathrm{SD}}$	*t*/s
AR M5P	0·0124	0·0003	0·0065	0·0001	0·0148	0·0009	0·0071	0·0002	1799
Bg M5P	0·0148	0·0001	0·0079	0·0001	0·0166	0·0008	0·0084	0·0002	3492
Dg M5P	0·0176	0·0003	0·0096	0·0002	0·0189	0·0014	0·0100	0·0002	117
Bg SVM	0·0315	0·0001	0·0194	0·0001	0·0314	0·0003	0·0195	0·0001	396 000
AR MLP	0·0339	0·0003	0·0237	0·0003	0·0336	0·0004	0·0236	0·0002	4000
Dg SVM	0·0336	0·0002	0·0218	0·0001	0·0337	0·0004	0·0218	0·0002	93 000
Bg MLP	0·0376	0·0003	0·0263	0·0002	0·0378	0·0008	0·0263	0·0004	20 000
Dg MLP	0·0382	0·0003	0·0268	0·0002	0·0380	0·0004	0·0267	0·0002	6243
AR LR	0·0477	0·0003	0·0351	0·0001	0·0473	0·0007	0·0349	0·0003	194
AR LMSQ	0·0481	0·0001	0·0350	0·0001	0·0475	0·0001	0·0348	0·0001	33 156
Bg LR	0·0475	0·0002	0·0350	0·0001	0·0476	0·0005	0·0350	0·0002	151
Bg LMSQ	0·0484	0·0002	0·0349	0·0001	0·0476	0·0005	0·0342	0·0002	94 949
Dg LR	0·0475	0·0002	0·0350	0·0001	0·0478	0·0005	0·0352	0·0003	17
Dg LMSQ	0·0482	0·0003	0·0351	0·0001	0·0484	0·0005	0·0351	0·0002	1357
AR SVM	0·0510	0·0003	0·0413	0·0001	0·0511	0·0006	0·0419	0·0002	8608

Table 5 Results of modelling process of MLP models predicting for *THC1* (sorted by $\mathrm{RMSE}_{\mathrm{val}}^{\mathrm{ME}}$) (source: Martínez-de-Pisón *et al.*[52])

	Training errors				Validation errors				
Algorithm	$\mathrm{RMSE}_{\mathrm{tr}}^{\mathrm{ME}}$	$\mathrm{RMSE}_{\mathrm{tr}}^{\mathrm{SD}}$	$\mathrm{MAE}_{\mathrm{tr}}^{\mathrm{ME}}$	$\mathrm{MAE}_{\mathrm{tr}}^{\mathrm{SD}}$	$\mathrm{RMSE}_{\mathrm{val}}^{\mathrm{ME}}$	$\mathrm{RMSE}_{\mathrm{val}}^{\mathrm{SD}}$	$\mathrm{MAE}_{\mathrm{val}}^{\mathrm{SD}}$	$\mathrm{MAE}_{\mathrm{val}}^{\mathrm{ME}}$	*t*/s
MLP *h*=40	0·0303	0·0020	0·0211	0·0021	0·0305	0·0020	0·0212	0·0022	52 167
MLP *h*=10	0·0308	0·0008	0·0209	0·0008	0·0309	0·0009	0·0210	0·0008	9958
MLP *h*=35	0·0306	0·0029	0·0213	0·0031	0·0311	0·0033	0·0214	0·0032	34 582
MLP *h*=07	0·0313	0·0004	0·0216	0·0006	0·0317	0·0007	0·0217	0·0006	9932
MLP *h*=05	0·0325	0·0004	0·0225	0·0003	0·0328	0·0007	0·0226	0·0003	7401
MLP *h*=03	0·0355	0·0005	0·0252	0·0003	0·0356	0·0005	0·0252	0·0004	3643



5 $RMSE_{val}^{ME}$ versus $RMSE_{tst}^{ME}$ for models evaluated



6 Comparative percentages of computation costs (t) for modelling 10 models: models discarded due to t>50 000 s are shown in boldface; label 'others' includes all other models with t<10 000 s

approaches. This paper also provides support for adjusting MLPs using LMS instead of least mean log squares (LMLS) as the error criterion because LMS costs three times less in terms of computation than LMLS for similar results.

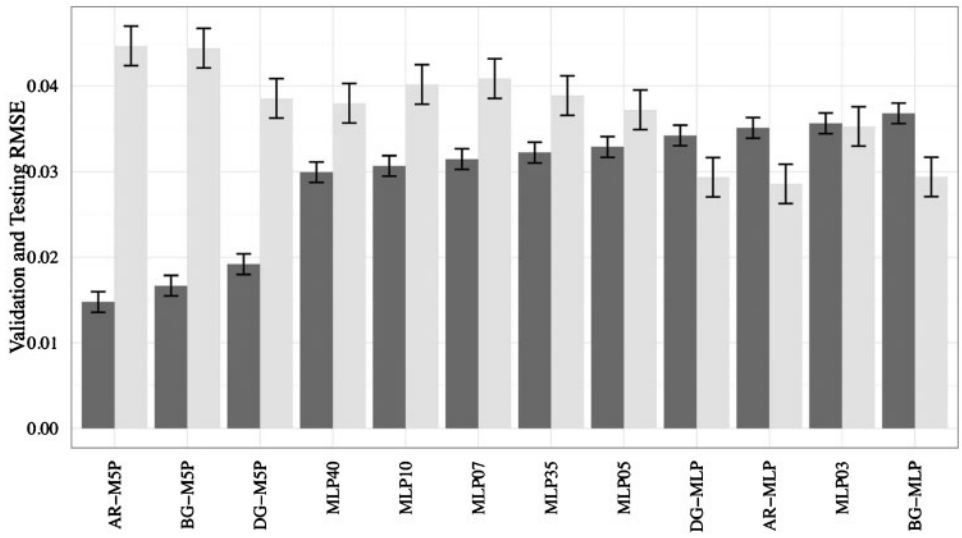
First, Table 4 shows that $RMSE_{val}^{ME}$ was <1·9% for every EM using M5P as its BL. Indeed, the $RMSE_{val}^{ME}$ values of M5P models, marked as group A in Fig. 5, are significantly lower than the rest. This suggests that the application of any ensemble scheme to a tree based regressor generates large models composed of several specialised trees with hundreds of leaves. These results contrast with those obtained from EMs that include MLP or SVM as their BL (except AR-SVM), marked as group B in Fig. 5, with $RMSE_{val}^{ME}$ ~3·5%. Table 4 also shows that the application of any ensemble scheme has a great influence on $RMSE_{val}^{SD}$ and MAE_{val}^{SD}, in terms of reducing them in comparison to the corresponding BL. AR-SVM and all the EMs that include LSMQ or LR as their BL (*see* group C in Fig. 5) present a $RMSE_{val}^{ME}$ higher than the predefined threshold $RMSE_{val}^{TH}=4{\cdot}0\%$. Thus, they fail to assure enough accuracy in predicting temperature THC1 and are therefore discarded.

In the next step (step 2), the time for training models is evaluated to check that they are generated in a time that is reasonable in proportion to the size of the modelling task. The time limit for training $M=10$ models (t^{TH}) is set at 50 000 s. Both Tables 4 and 5 show that the computation costs associated with SVM based EMs and those MLP based EMs with high numbers of neurons in the hidden layer ($h=40$) are higher than t^{TH}. For that reason, bagging SVM, dagging SVM and MLP with $h=40$ are automatically discarded. Note that the computation times for the training phase summarised in Table 5 differ from the results previously published because the simulations are repeated to gather new times in equal conditions for all models. The comparative percentages are shown in Fig. 6 to highlight significant differences between algorithms. However, the BLs that make up EMs can be independently trained in parallel, drastically decreasing the training time of EMs.

The model's reliability in predicting THC1 from unseen data is analysed in step 3. Table 6 shows the testing errors of a number of $M=10$ models with the setting parameters that generate the lowest $RMSE_{val}^{ME}$. It is observed that the best performing of all the models in Step 1 provides the worst results in step 3, i.e. $RMSE_{tst}^{ME}$ of M5P based EM is higher than 4·5% when $RMSE_{val}^{ME}$ was <1·9% in step 1. We illustrate $RMSE_{val}^{ME}$ and $RMSE_{tst}$ together in Fig. 7 to support the selection of the best overall models. The error bars represent least significant difference values to visually identify whether an error is significantly lower than others. The figure leaves no doubts that M5P based EM shows the lowest generalisation capacity when working with new coils and, conversely, MLP with only three neurons in the hidden layer (MLP03) and MLP based EM (AR MLP, Bg MLP and Dg MLP) are the best overall models. The main reason is that these last four models show high capacities to achieve a good balance between validation and testing errors because their structure is less complex

Table 6 Testing errors of THC1 prediction models (sorted by $RMSE_{tst}^{ME}$), including MLP models from previous article (source: Martínez-de-Pisón *et al.*[52])

Algorithm	$RMSE_{tst}^{ME}$	$RMSE_{tst}^{SD}$	MAE_{tst}^{ME}	MAE_{tst}^{SD}	CV
Dg MLP	0·0284	0·0003	0·0218	0·0004	0·0106
Bg MLP	0·0294	0·0003	0·0233	0·0002	0·0102
AR MLP	0·0298	0·0001	0·0228	0·0002	0·0034
MLP h=07	0·0322	0·0019	0·0241	0·0016	0·0590
MLP h=03	0·0322	0·0019	0·0249	0·0018	0·0590
Bg SVM	0·0329	0·0001	0·0241	0·0002	0·0030
Dg LR	0·0332	0·0001	0·0258	0·0001	0·0030
AR LR	0·0332	0·0003	0·0257	0·0002	0·0090
Bg LR	0·0333	0·0001	0·0258	0·0001	0·0030
Bg LMSQ	0·0334	0·0001	0·0262	0·0001	0·0030
ARLMSQ	0·0348	0·0009	0·0278	0·0008	0·0259
MLP h=05	0·0361	0·0044	0·0274	0·0041	0·1219
Dg SVM	0·0364	0·0007	0·0273	0·0006	0·0192
MLP h=40	0·0368	0·0017	0·0274	0·0013	0·0462
MLP h=35	0·0378	0·0019	0·0281	0·0014	0·0503
MLP h=10	0·0390	0·0026	0·0289	0·0018	0·0667
Dg LMSQ	0·0452	0·0052	0·0289	0·0013	0·1150
AR M5P	0·0458	0·0059	0·0303	0·0029	0·1288
AR SVM	0·0465	0·0002	0·0377	0·0002	0·0043
Dg M5P	0·0497	0·0136	0·0293	0·0034	0·2736
Bg M5P	0·0610	0·0009	0·0299	0·0001	0·0106



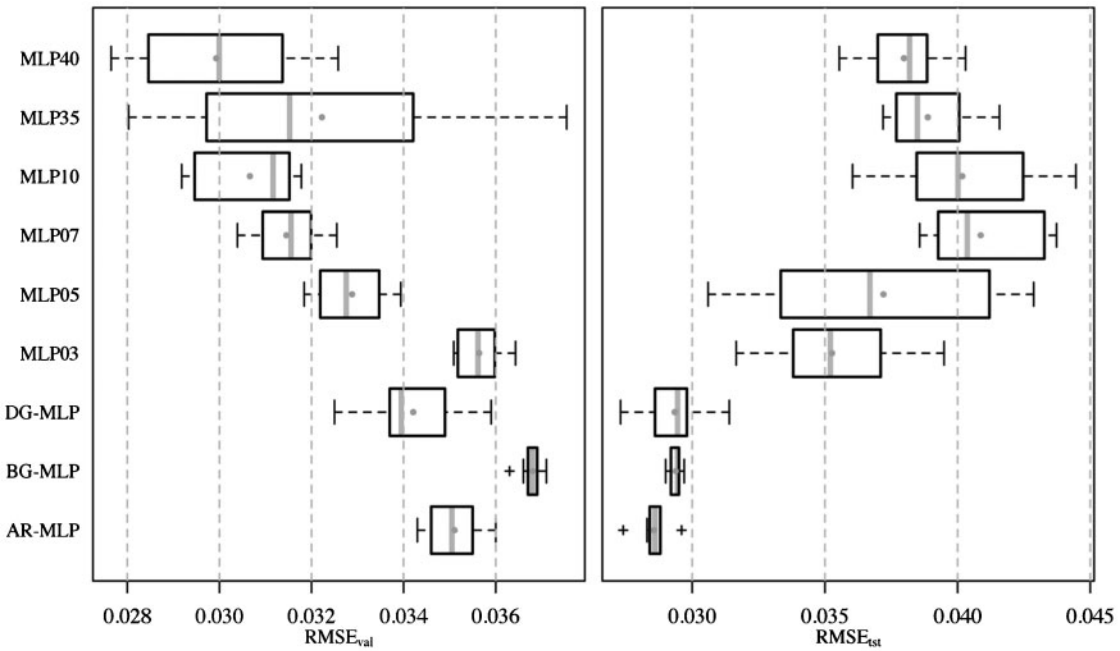
7 Bar plot with error bars of $RMSE_{val}^{ME}$ and $RMSE_{tst}^{ME}$: dark and light grey bars correspond to validation and testing errors respectively; error bars represent least significant difference between means; thus, two overlapping bars indicate non-significant difference and non-overlapping bars indicate opposite

and not so specialised in coils already treated. Moreover, some models sometimes present lower $RMSE_{tst}^{ME}$ than $RMSE_{val}^{ME}$ because the validation dataset may be more complex than testing dataset.

Finally, the stability of models is measured and compared by determining the $RMSE_{tst}^{SD}$ and CV_{tst}. Stability is formally defined as the degree to which a technique creates repeatable results, given different datasets sampled from the same data. The aim is to find those models that have the lowest $RMSE_{tst}^{SD}$ and CV_{tst} at the same time. Models are not very reliable if they predict different values each time there are slight changes in the input data or even in some of the setting parameters of the model itself. Table 6 shows that EMs that use MLP as BL are the more stable because their CV_{tst} are at least four times lower than each single MLP. Additionally, Fig. 8 lends support to previous observations by illustrating $RMSE_{tst}$ as a box plot of the testing error distribution. It can be claimed that EMs using MLP as BL have a narrower $RMSE_{tst}$ distribution than any single data driven model.

Conclusions

This paper mainly presents three ensemble schemes that combine the outputs of several data driven models to predict temperature set points for a CAF on an HDGL. The main contributions relate to the description of a methodology for evaluating models, the comparative evaluation of 15 cases and the final recommendations



8 Box plots of RMSE (left, validation; right, testing): whiskers cover those samples that are outside interquartile range but are not outliers; crosses represent outliers that are samples at distance of >1·5 times interquartile range; grey dots and grey lines are mean and median of data respectively

for using ensemble learning as a regression technique. Ensemble methods generally show themselves to be highly efficient and reliable in terms of computation cost, generalisation capacity and ease of determination of the best model configuration. However, comparative evaluation proves that the use of MLP as BL is the best choice for generating the best performing model, i.e. AR MLP, Bg MLP and Dg MLP. Compared to single MLP, MLP based EM achieves similar accuracy in predicting temperature set points for types of coils stored in the modelling DB but a lower generalisation error with coils not previously processed. This demonstrates that EMs are universal in nature and better suited for working with low quality and sparse DBs from industrial processes. Finally, the extra cost in computation time required for these models is not so restrictive if it is considered that they can be easily parallelised and plant engineers can also avoid continually having to change the model for new products thanks to its higher overall capacity and stability.

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Chapter 6

Results

This chapter reports the results related to the contributions made by this thesis. From a general perspective, these results are a guide for understanding the objective criteria that evaluate the possibilities of DM and SC techniques for discovering useful knowledge. We seek a better understanding of galvanising lines in order to improve their performance. We have thus obtained knowledge in the form of association rules and prediction models.

An outline of the overall results is presented first, followed by detailed descriptions of the specific results obtained with each methodology in the separate sections below.

The first section shows a list of rules generated by our work for explaining frequent failures detected in a galvanising process. The study was based on a DB created during the first adjustment tests for a new type of steel at the plant. When dealing with new products, there are many drops in the quality of the zinc coating due to the difficulty that plant engineers encounter when adjusting all the process parameters. The conventional processing of TS cannot provide such accurate information on these failures. First, our overall methodology reduced the number of rules that appeared as possible candidates. Surprisingly we found two useful non-trivial rules that proved to have a close link to the failures once they had been evaluated by plant experts.

The second and third sections describe two studies on developing overall parsimonious models based on non-parametric regression methods. In particular, MLP models and MLP-based EMs, which were consistent with previous studies

recorded the lowest generalisation errors with a highly stable prediction of novel data from the CHDGL. These results reveal a reduction in the problems of over-fitting, excessive complexity of models and the curse of dimensionality in their inputs. In addition, they enhanced our previous work on non-linear modelling, so the resulting models had the highest scope for being both comprehensive and parsimony.

The specific results relating each contribution in this thesis are throughly described below to provide detailed information on the performance of our methodologies and the models generated.

6.1 Results in Publication I

All the results described in this section are presented in the paper "*Mining association rules from time series to explain failures in a hot-dip galvanising steel line*" (Martínez-de Pisón *et al.*, 2012).

Our aim was to validate the methodology employed using data with information from a batch of 723 coils of a new type of steel. We thus carried out an experimental evaluation. 5.4 % (39) of these coils were found to contain irregularities in the adherence of the zinc coating layer. This percentage of coils with uneven adherence is relatively high because the dataset was collected during the first adjustment tests at the plant.

The first step provided in a selection of TS corresponding to the mean of the readings taken for 100 meters of steel strip that could have crucial influence on the galvanising process. The features selected were (1) the concentration of H_2 and (2) the concentration of O_2 in the air composition in a specific zone, (3) the temperature in each zone, (4) the strip velocity, (5) its temperature (measured with a pyrometer in each area), (6) the dew point temperature in each zone, (7) the width and (8) thickness of coils, (9) the chemical composition of the steel in each coil, and finally (10) the temperature and (11) composition of the zinc bath (Table 1, 2 and 3, Martínez-de Pisón *et al.*, 2012). There was a single logical output to indicate whether or not the thickness of the zinc coating was acceptable. The variables were filtered in the next step to remove zero or very low values due to data gathering failures or sensor deficiencies. Maxima and minima were also obtained in the same step with a view to extracting the significant events later. A total of 120 types of significant events were deemed useful for

discovering knowledge.

The dataset of $E = 39$ transactions of significant episodes occurring prior to the adherence failure of the zinc coating was created by using a time window width of 80 ut and a time lag of zero. Setting the consequent *Conseq* to "ADHERENCE_BAD" as the detection of a failure due to poor adherence, a search was preformed with the ECLAT algorithm (Zaki, 2000) for those frequent episodes recorded over the preceding 8 000 m of strip. The critical parameter *RelSupportWinRule* was set to 50 % and a total of 64 frequent episodes were identified with different *RelConfidenceWinRule* for each one of the rules extracted using the same consequent (*Conseq*=ADHERENCE_BAD).

The first 20 rules extracted with maximum *RelSupportWinRule* were reported (Table 4, Martínez-de Pisón *et al.*, 2012). They included many redundant rules with different values of *RelConfidenceWinRule,* showing the number of times that the antecedent appears when a faulty zinc coating occurs, divided by the number of times that the antecedent appears within the predefined window. Surprisingly, while the number of redundant rules was large in comparison with the total number of rules found, the complexity of the two rules selected was high enough for our purposes. Therefore, the "interesting" rules to be analysed were the two rules with the highest *RelConfidenceWinRule*, which were highlighted in bold in Table 4 (Martínez-de Pisón *et al.*, 2012)

[3] IF {(BATH_TMP_BELOW) & (SPD_DEC) & (ZO6_TMP_BELOW)}

THEN ADHERENCE_BAD $[WinW = 80, TimeLag = 0]$

RelSupportWinRule=67%, *RelConfidenceWinRule* =76%

[15] IF {(BATH_TMP_BELOW) & (SPD_NOT_HOR) & (TMP_PO2_BELOW)}

THEN ADHERENCE_BAD $[WinW = 80, TimeLag = 0]$

RelSupportWinRule = 62% , *RelConfidenceWinRule* = 80%

The detailed explanation about the interesting rules selected is as follows

1. The first association rule occurred with 67 % of database T, and the consequent was fulfilled 76 % of the times when the antecedent appeared. In other words, this rule is fulfilled 67 % of the times when there has been an

adherence fault. Furthermore, it is a rule with a high confidence level, as 76 % of the times when the antecedent has occurred there has also been an adherence fault. The rule indicates that when the temperature in the zinc bath is low (`BATH_TMP_BELOW`), the temperature in zone 6 of the furnace is also low (`Z06_TMP_BELOW`) and the strip feed rate falls sharply (`SPD_DEC`), then resulting in a faulty zinc coating (*Conseq*=`ADHERENCE_BAD`).

2. The second association rule reveals that when sudden changes in velocity (`SPD_NOT_HOR`) occur together with low zinc bath (`BATH_TMP_BELOW`) temperatures and low strip temperatures at the furnace outlet (`TMP_P02_BELOW`), errors in the zinc coating result. In this second case, this occurred 80 % of the time. In other words, 62 % of the faulty coils are preceded by the episodes described in this rule. In addition, 80 % of the times this antecedent has occurred there have also been coating faults on the coils.

In short, like the majority of research on ARM, the rest of the rules discovered described almost the same episodes than the two rules outlined before. However, these redundant rules cannot be marked as interesting as their *RelConfidenceWinRule* values are too low.

6.2 Results in Publication II

All the results summarised in this section are presented in the paper "*Methodology based on genetic optimisation to develop overall parsimony models for predicting temperature settings on an annealing furnace*" (Sanz-García *et al.*, 2012). Overall, the results presented below provide enough evidence to support the practical use of the methodology proposed for generating overall parsimonious models.

The different series of experiments were carried out using solely MLPs based on prior experiences and acquired knowledge (Fernández-Ceniceros *et al.*, 2012; Martínez-De-Pisón *et al.*, 2006, 2011). The search for overall parsimonious MLP models for predicting three temperature set points on a CAF (*THC1*, *THC3* and *THC5*) was the main step in the proposed methodology based on GAs. The maximum number of generations of the ending condition G was 50, and the number of individuals in population P was limited to 50. A binary chromosome of 39 bits was defined for finding the optimal values of model parameters within following ranges: $H := \{2 : 50\}$, $\eta := \{0 : 1\}$, $M := \{0 : 1\}$ and $q_j := \{2^0 - 1 : 2^{19} - 1\}$. Other parameters were set during the process, such as 1000 for the maximum

number of epochs for training models. Additionally, several prior trials were previously conducted to gain insight into the process adjustments. The following suitable values were found for the configuration parameters of the GA: elitism percentage $x_e = 20\,\%$, mutation factor $\chi = 39^{-1}$ and crossover proportion of $50\,\%$. An ESC was also set up in the same experiments as follows: fraction for adjusting penalty function $x_g = 0.2$, weighting coefficient of the complexity term $\mu = 0.02$, period of stability $T_g = 10$ generations, $I = 10$ best individuals per generation and percentage $x_{val} = 0.01\,\%$ for $x_{CI} = 90\,\%$.

In the case study involving the prediction of three temperature set points on a CAF, the MLP developed with the proposal performed better than those without it. On the one hand, the testing errors ($RMSE_{tst}$) for the best models using optimisation with a complexity function did not exceed $4.5\,\%$ (Table 1, Sanz-García *et al.*, 2012). These models had similar or slightly higher validation errors ($RMSE_{val}$) than the others, but significantly lower $RMSE_{tst}$ values predicting both *THC1* and *THC5* temperature set points (for *THC3*, the $RMSE_{tst}$ was similar to the method without complexity function). On the other hand, Pearson's correlation coefficient (R^2) was included to evaluate linear dependence between measures and model predictions. The R^2 testing of the MLPs in our proposal clearly records values which better than or equal to those obtained when the complexity function is omitted.

Interestingly, models trained with complexity control showed a greater capability for generalisation in two cases (*THC1* and *THC5*), i.e. $RMSE_{val}$ was equal to or even higher than $RMSE_{tst}$. However, no significant difference was found between *THC3* prediction models with and without complexity function. The most striking result was the lowest $RMSE_{tst}$ ($3.29\,\%$) of the *THC5* prediction model using the complexity function that reinforces the usefulness of the proposal. These interesting results were consistent with the number of neurons in the hidden layers of the models. The models trained with complexity control had a total number of neurons equal to or even lower than the models developed without our proposal (Table 1, Sanz-García *et al.*, 2012). These findings are a clear consequence of the model´s reduced number of setting parameters.

The representation of the evolution of $RMSE_{val}$ and $RMSE_{tst}$ across the optimisation process with and without complexity control was crucial to confirm the abovementioned results (Figures 9 to 14, Sanz-García *et al.*, 2012). As observed, both errors were stable and of the same order of magnitude in the last generation in Figures 10, 11 and 13. By contrast, Figures 9, 12 and 14

(Sanz-García *et al.*, 2012) show three processes in which the best solution was not achieved in the last generation. It is essential to note that the distinction between the use and non-use of a complexity function is shown in Figures 11 and 14. The most remarkable result to emerge from both figures is that there was no possibility of finding a subset of steady setting parameters for *THC5* prediction models without including the complexity term in the fitness function (J) of the GA.

All the plots in Figure 15 (Sanz-García *et al.*, 2012) were also consistent with previous findings, which represents errors via the aggregation coefficients W of models. Figure B.3, Figure B.4 and Figure B.5 extend the range of W from 30 to 50, providing more information. First, Figures 15.a and 15.b show $RMSE_{val}$ and $RMSE_{tst}$ predicting *THC1* against the complexity function over generations with and without complexity control, respectively. Figures 15.c and 15.d represent the same results for the case of *THC3* and, finally, *THC5* corresponds to Figures 15.e and 15.f. Second, the balance between $RMSE_{val}$ and $RMSE_{tst}$ predicting *THC1* is higher in Fig. 15.a than in Fig. 15.b because the penalty function reduced the number of overfitted models. In the case of temperature *THC3*, Fig. 15.d shows a lower density than Fig. 15.c in the lower part of the plot, which means a sharp reduction in computation cost. All these findings are also repeated in Figure B.3, Figure B.4 and Figure B.5. Our methodology including the complexity function and an ESC has a clear advantage over standard GAs in Figure B.5 due to the low density of grey points ($RMSE_{tst}$) identified in the lowest values of both axes.

The ESC also reduced the total computation cost for training models (Table 1, Sanz-García *et al.*, 2012). Our results confirms that the performance of the resulting models did not decrease, while total computation costs were lower in two of the three cases studied (Figures 9 to 14, Sanz-García *et al.*, 2012). Nevertheless, the importance of including an ESC appeared surprisingly in Figure 9, when the best individual in the last generation was not the best model trained. Figure 9 revealed that the generalisation error of the *THC1* model trained including the complexity term in J increased from the 30^{th} generation to the last. In short, Figures 9, 10 and 11 show that we stopped the uncontrolled overfitting. They offer evidence for considering a key requirement in the combination of the complexity control and the ESC.

A comparison between the results in the best models obtained (see Table 1, Sanz-García *et al.*, 2012) and the number of the total inputs selected by the GA-based feature selection (FS) (Table 2, Sanz-García *et al.*, 2012) also shows

that working on a reduced set of attributes has additional benefits. Figure 16 (Sanz-García *et al.*, 2012), Figure B.1 and Figure B.2 show the evolution of the selected inputs in *THC1*, *THC3* and *THC5* prediction models, respectively, for the 10 best individuals over 50 generations; in other words, they present each variable's significance in the accuracy of the 10 best models per generation. In those figures, the stopping generation is represented using a triangle when the input was not finally selected and an inverted triangle in the opposite case.

Figure 16 (Sanz-García *et al.*, 2012) shows that the final model trained with the complexity penalty was developed using only four inputs, and the one trained without the complexity function had eight inputs; which is the same as saying that obtained half as much complexity in final models with the proposed complexity control as in those without it. Both methods chose the inputs *VelMed*, *ThickCoil* and *TMPP2CNG*, but the one with complexity control only additionally selected *P*, while the standard method added attributes *C*, *Si* and *Mn*.

Lastly, a set of attributes stemming from chemical components such as *Cu*, *B*, *N* and *V* reflect far less variation in models optimised with the complexity function than in those without it. Other inputs such as *ThickCoil*, *TMPP2CNG* and *VelMed* were always significant, so maintaining these attributes as inputs enhanced the accuracy of the resulting models. A more detailed analysis of these figures shows that *TMPP1* and other chemical components such as *Al*, *Nb* and *Ti* were never selected. These findings offer compelling evidence for concluding that our proposal with the complexity term rendered it easier to remove irrelevant inputs, enhancing the stability of the optimisation process.

6.3 Results in Publication III

All the results described in this chapter are included in the article "*Overall models based on ensemble methods for predicting continuous annealing furnace temperature settings*" (Sanz-García *et al.*, 2013).

The steps and criteria of the methodology proposed were applied to models predicting three temperature set points *(THC1*, *THC3* and *THC5)* for a CAF on a CHDGL. However, we report only those results concerning 15 different types of models predicting *THC1*. The results of *THC3* and *THC5* prediction models (30) differ so slightly from those of *THC1* that we can suitably summarise the

entire information on the evaluation simply by studying *THC1* results.

In brief, the prediction models trained were based on three ensemble schemes as follows: (1) additive regression (Friedman, 1999), (2) bagging (Breiman, 1996), and (3) dagging (Ting, K. M., 1997). Additionally, the five basic components of the three EMs selected were the following data-driven models: (1) least median squared linear regression (LMSQ) (Rousseeuw & Leroy, 1987), (2) linear regression (LR) (Burnham & Anderson, 1998), (3) Quinlan´s improved M5 algorithm (M5P) (Wang & Witten, 1997), (4) MLP networks (Haykin, 1999), and (5) SVMs (Smola & Schölkopf, 2004). We wanted to explore different configurations within a limited number of trials (Tables 2 and 3, Sanz-García *et al.*, 2013). We thus generated different models using ranges for the values of the pre-established setting parameters.

By applying an iterative training process, the results of the evaluation based on the methodology proposed were obtained, together with the resulting models. As the main component of the methodology, the evaluation was organised according to the following criteria: the computation cost of training N_{tr} models (t), the root mean squared error ($RMSE$) and mean absolute error (MAE) in validation and testing process, and the coefficient of variation (CV) that measures model stability by comparing the amount of variance between sets with different means. Model stability is important for indicating the degree to which a technique creates repeatable results for different datasets sampled from the same raw dataset.

Overall, the results are summarised in three tables (Tables 4, 5 and 6, Sanz-García *et al.*, 2013). Table 4 presents a significant difference between the training and validation errors of *THC1* prediction models based on EMs; Table 5 reports less variation between the training and validation errors of the MLP models (Martínez-De-Pisón *et al.*, 2010b); and finally, Table 6 presents the most important difference between the testing errors of the two ensembles and MLP models.

As expected in tree-based regressors, our evaluation shows that the application of any ensemble scheme to M5P generates large models composed of several specialised trees with hundreds of leaves with significantly lower validation errors than the rests ($RMSE_{val} = 0.0148 \pm 0.0009$ and $MAE_{val} = 0.0071 \pm 0.0002$, $mean \pm sd$). These results contrast with those obtained from EMs that include MLP or SVM as their base learner (BL) (except AR-SVM) with higher validation errors ($RMSE_{val} \geqslant 0.0314 \pm 0.0014$ and $MAE_{val} \geqslant 0.0195 \pm 0.0002$). However,

taking the EMs as a whole, our results show that the application of any ensemble scheme has a great influence on the standard deviation of the validation errors, in terms of reducing it in comparison to the corresponding BL reported by Martínez-De-Pisón *et al.* (2010b).

Likewise, the training time (t) of the resulting models was evaluated to check that models were adjusted in a time that was reasonable in proportion to the size of the modelling dataset (Figure 6, Sanz-García *et al.*, 2013). The time limit for training $N_{tr} = 10$ models was directly related to the size of the training dataset; and although its value could not be optimal, the limit was established at $t = 50\,000$ s. The significant differences between different EMs were readily highlighted by using comparative percentages of the total training times. As expected, the experiments proved that the computation costs associated with SVM-based EMs and MLP-based EMs with high numbers of neurons in the hidden layer were the highest of all ($t > 50\,000$ s).

The reliability of the models in predicting THC1 from unseen data was also analysed in the next step (Figure 7, Sanz-García *et al.*, 2013). The best-performing model in the validation process, which corresponds to the first step, provided the worst results in the testing process, i.e. M5P-based EMs had a testing error of $RMSE_{tst} = 0.0458 \pm 0.0059$ and $MAE_{tst} = 0.0303 \pm 0.0029$, whereas the same model recorded the lowest validation errors of all the models ($RMSE_{val} = 0.0148 \pm 0.0009$ and $MAE_{val} = 0.0071 \pm 0.0002$) with the same setting parameters. This phenomenon is graphically represented in the paper, leaving no doubts that M5P-based EMs have the highest generalisation errors when working with new coils and, conversely, MLPs with only three neurons in the hidden layer (MLP03) and MLP-based EMs (AR-MLP, BG-MLP and DG-MLP models) are the models with the lowest generalisation errors.

Finally, we sought to find those models with the lowest $RMSE_{tst}^{SD}$ and CV_{tst} at the same time. We thus evaluated model stability by comparing $RMSE_{tst}^{SD}$ and CV_{tst}. The results of the evaluation clearly show that the values for MLP-based EMs are at least four times lower than each single MLP model (Table 6, Sanz-García *et al.*, 2013) and, therefore, the MLP-based EMs show much greater stability (Figure 8, Sanz-García *et al.*, 2013).

Chapter 7

Discussion

This chapter presents the theoretical and practical implications of this work, its limitations and possible topics for further research. The chapter is organised following the same sequence as the results (see Chapter 6).

The main goals of this thesis were to seek useful non-trivial rules and find out which predictive non-parametric methods would be useful and feasible for producing overall parsimonious regression models from large volumes of industrial DBs.

As an initial contribution, the main goal was to extract valuable knowledge in the form of association rules to reduce the adherence defects affecting the zinc coating on a CHDGL.

The most striking result that emerged from the data was the extraction of two rules with very high *RelSupportWinRule* and *RelConfidenceWinRule* values. According to the opinion of the plant experts, both rules were useful for identifying the causes of adherence failure in a significant percentage of defective coils. Thus, we believe that this is solid proof that the methodology is capable of discovering useful hidden knowledge.

Under particular circumstances, this knowledge could also help technicians to evaluate the impact of the process variables on the adherence of the zinc coating. Moreover, it could even help to identify which parts of the process should be the focus of corrective and surveillance actions. The parts can be identified

by analysing all the frequent episodes and the variables that define these.

As expected, the pre-processing phase is highly dependent on eliminating spurious data, but the experiments also show that some steps in the methodology depend heavily on the expertise of analysts and engineers. For instance, extreme caution should be taken when determining the threshold values for the parameters in Step 2 in which the minima and maxima are obtained. This can be considered as one of the most critical points in iterative TS processing due to the sensitivity showed by the parameter R (Fink & Pratt, 2004). In conclusion, the "human factor" is still vital at several steps in this methodology.

Curiously, the combination of ECLAT, a widely-known algorithm with a pre-set window and a time lag between the window and the failure to explain (or consequent of the association rule), generated efficient tools for extracting rules from the dataset. On the one hand, the use of ECLAT speeded up the search process and rendered it not necessary to look for more complex algorithms. On the other hand, the combination of ECLAT and the sliding window enhanced the efficiency and also the speed of the process because of the drastically reduced size of the data.

Our experiments were performed using a window width and a time lag, maintaining both parameters at low values. This allowed us to reduce the size of the original dataset, with the effect being an increase in the performance of *RelSupportWinRule* and *RelConfidenceWinRule*. We conclude that we made a good choice in the parameter setup because the causes of the failures tended to be relatively close in time to the moment of the failure in most of the industrial processes. It should be noted that low values of *RelConfidenceWinRule* always indicate a weak relation between the antecedent and the consequent, as the antecedent appears regardless of whether or not the consequent occurs; by contrast, a high value of *RelConfidenceWinRule* indicates a cause-effect relationship between the antecedent and the consequent. If a good performance is desired, the methodology needs to maintain both *RelSupportWinRule* and *RelConfidenceWinRule* at very high values.

Apart from the previous two rules described in Chapter 6, we found others with very high *RelSupportWinRule* (see Table A.1, Table A.2 and Table A.3). This tends to happen when the DB contains large volumes of trivial information and leads to the existence of many redundant episodes with high *RelSupportWinRule*. Some of these rules were automatically discarded, as they were deemed to be weaker than the two initial rules because of their lower *RelConfidenceWin-*

Rule. However, the remaining rules were not finally selected due to the experts´ decision based on their experience in the field. Obviously, the methodology is not capable of automatically separating useful rules from redundant ones. As this selection could be highly subjective and depends on the experience of the experts involved, our findings need to be interpreted with caution, as other potentially useful rules may still remain in the dataset.

Our methodology reproduced the hidden knowledge properly using the types of event proposed. We believe that these events were very easy to understand and use, and they also struck the right balance between information provided and complexity. Nevertheless, according to the previous paragraph, the need for manual adjustment was once again crucial. Plant's technicians and additional information from previous papers helped to take the final decision on the number of variables to be included in the study. In addition, the values of the search parameters for each one of the events were defined again, with the help of on-site technicians.

According to Mannila (1997), the purpose of DM is to extract useful information from large volumes of data, a task that has traditionally been a manual procedure. Due to the exponential increase in the sizes of databases, there is a need to propose novelty automated methodologies for this task. Nevertheless, a fully automated methodology cannot be expected to work properly, since an expert in the field is required, for instance, to judge the relevance of the findings.

We are aware that the methodology may have other limitations. The most important one is that it is not possible to estimate how many rules may still be hidden. A further limitation is that we do not know whether the rules discovered include all the attributes that explain the adherence defects affecting the zinc coating. Taken as a whole, the methodology provides useful knowledge but it is relatively limited because there is no automatic quantification of the importance or richness of the rules.

On a practical level, the conclusion drawn is that by means of iterative and interactive adjustments of the pre-processing and segmentation functions (filters, detection of significant maxima and minima, definition and extraction of episodes) experts can obtain significant rules more reliably than with fully automatic rule extraction systems. We therefore consider it worthwhile to make the effort required to develop tools to facilitate iteration for experts and analysis software in all pre-processing and time series segmentation tasks.

It should be noted that the episodes used were only of a "serial" type because they are easy to manage, although some failures in the process may be explained solely with parallel episodes. Thus, a future aim is to improve the methodology by using different type of episode that is more flexible, i.e. non-serial and non-parallel episode. Another interesting improvement may involve using the logic of fuzzy associations to seek more flexible sequences akin to human thought processes. The technique has already been proposed by Luo & Bridges for frequent episode mining to evaluate the performance of network intrusion detection systems.

All in all, the methodology applied to the process studied provides knowledge that can be used to identify both the main circumstances that affect the quality of the coating on the coils and the control actions that can be implemented as a safety measure to resolve the problems arising (Martínez-De-Pisón *et al.*, 2006; Alfonso-Cendón *et al.*, 2010)

The second contribution focuses on improving the prediction of setting parameters in continuous processes. The final goal was to develop a methodology for training overall parsimonious MLP models to predict three temperature set points (*THC1*, *THC3* and *THC5*) for a CAF on a CHDGL.

Our work centred mainly on validating the usefulness of the semiautomatic methodology proposed. Two characteristics distinguish our method from other optimisations based on GAs. Ours includes a complexity penalty in fitness function J and also an ESC in the optimisation process.

Note that the problem of developing overall parsimonious MLP networks is common place in computer science. It can be found in many rigorous studies published in the field (Schaffer *et al.*, 1990; Chellapilla & Fogel, 1999; Norgaard *et al.*, 2003; Jones *et al.*, 2005; Siwek *et al.*, 2009; Agarwal *et al.*, 2010). The goal is to provide a higher capacity to increase the model´s generalisation capability.

Overall models are those that should not only have a suitable prediction capacity regarding known data, but also be accurate when predicting novel data. These models were obtained in the last generation of the optimisation process, as Figures 10, 11 and 13 (Sanz-García *et al.*, 2012) illustrate. Surprisingly, this did not occur in all the experiments. As we can seen in Figures 9, 12

and 14 (Sanz-García *et al.*, 2012), the best solution was not achieved in the last generation of these optimisation processes. This diversity clearly demonstrates that standard GA-based optimisation did not automatically generate the expected overall models. Over-fitting can be observed in the last models generated in Figures 9, 12 and 14 (Sanz-García *et al.*, 2012).

The first modification made to our methodology was to include the ESC. This is a supervisory control that can solve the overfitting problems during the optimisation process, especially when dealing with industrial data. The results in Table 1 (Sanz-García *et al.*, 2012) allow us to conclude that the generalisation capacity of the resulting models was enhanced. This statement is consistent with the literature (Chellapilla & Fogel, 1999; Islam *et al.*, 2001, 2003). Nevertheless, it must be remarked that in some cases (Figures 12 and 14, Sanz-García *et al.*, 2012) the control of the evolutionary process using the ESC did not suffice achieve our initial goals.

One solution to this problem is to include a complexity penalty in the fitness function J of the GA-based optimisation (Chaturvedi, 2008). Although the application of this solution has been satisfactory for small DBs, it can also be applied to complex DBs from industrial processes. We consider this crucial for determining its usefulness in the support of real industry objectives. As far as we know, this is currently under analysis.

We wanted to remove this limitation from the optimisation process, we included the term W in the fitness function J. Figure 11 (Sanz-García *et al.*, 2012) shows the effect of this term in comparison to Figure 14 (Sanz-García *et al.*, 2012), in which the complexity penalty is not used. We conclude that W guarantees the existence of at least one stable period to achieve more accurate results. The benefits of the inclusion of W in the fitness function J are due to the reduction in the number of neurons in the hidden layer of the MLP models. Models were less complex and, consequently, their training time is also reduced.

These results prove that our method can significantly decrease the risk of overfitting by training the MLPs in the cases in which it was applied. Consequently, we show that overall parsimonious models can be generated by using both the complexity term and the ESC. These findings are useful for reinforcing the application of this proposal in the steel industry.

A well-known disadvantage of using GAs is the need for massive data processing that always involves high computation costs (Goldberg, 1989). Just

as the complexity penalty was crucial for reducing the training time of models, the ESC has also turned out to be very useful for reducing the computation cost of the optimisation in two (*THC1* and *THC3*) of the three processes. In case of *THC5*, the best models were always found in the last generation. The reason for these rather contradictory results is still not entirely clear. We assume that the complexity of the DB may have some influence.

With no loss of model accuracy, total computation cost for training the models was always the same or lower using these parameters than without them. We conclude that the combination of both the two modifications (W and ESC) is an appropriate solution.

In a previous paper, Martínez-De-Pisón *et al.* (2010b) report substantial improvements in the reduction of the number of input variables related to chemical composition of steel by using principal component analysis (PCA) (Pearson, 1901; Hotelling, 1993). PCA has shown itself capable of transforming fourteen initial variables for the chemical composition of steel into a small set of seven uncorrelated inputs. The disadvantage of applying this technique is quiet clear. The interpretation of the resulting models is more difficult as raw variables are no longer being used.

GAs have been widely used for FS in a wrapper approach in many previous articles (Guerra-Salcedo & Whitley, 1999; Opitz, 1999; Tang & Honavar, 1997). In our method, GA-based FS has been used to create a subset of input variables from an initial set of all the variables without any exception. The results obtained (Table 1, Sanz-García *et al.*, 2012) show an increase in model accuracy using GA-based FS. The lower errors were due to a less collinearity between the data. This has also leads to higher parsimony in the models.

Consequently, the new method seems more suitable for selecting solely those variables needed to generate parsimonious models. The aim was to reduce the number of variables for the chemical composition of steel. We thus conclude that the use of GA-based FS has more advantages than PCA. In addition, it should be noted that GA-based FS is more robust than PCA because the former does not assume that the scores from its models must be normally distributed.

Our results also confirm that GA-based FS enhanced the interpretation of the final models. The interpretation of the selected variables can provide plant experts with more information about the annealing treatment and the influence certain particular variables have on it. Using our methodology makes it easier to

find the most significant variables for generating more parsimonious models.

The inputs *VelMed*, *TMPP1*, *WidthCoil*, *ThickCoil* and *TMPP2CNG* were included in the models from a previous paper (Martínez-De-Pisón *et al.*, 2010b) with no prior significance rating. In our methodology, *VelMed*, *ThickCoil* and *TMPP2CNG* are also maintained as inputs, so these attributes clearly enhance model accuracy. These statements are consistent with previous research, where these are the only inputs to have been selected (Martínez-De-Pisón *et al.*, 2010b). However, in this thesis, *TMPP1* was always discarded in all cases. One conclusion is that *TMPP1* is redundant and not therefore relevant for use as an input.

The input TMPP1 was discarded together with *Al*, *Nb* and *Ti*, which finally became irrelevant attributes forthcoming from chemical composition. The inputs *C*, *Si* and *Mn* have the same performance together as the first model with only the variable *P*. This shows that both fitness functions can produce high performance models, but only our proposal generates a parsimonious model. In these cases, according to Guyon & Elisseeff (2003), some variables that are useless by themselves can be useful together. A similar behaviour has been observed for *THC3* and *THC5* prediction models (see Supplementary Material in Sanz-García *et al.*, 2012).

We are aware that our methodology has two main limitations: the first is that it is not as fully automatic as we would have linked. The starting operations for setting the parameters of the optimisation process are not automatically performed. Iterative work is always required to achieve good results. This apparent lack of automation at the starting point means that the method is finally classified as semiautomatic. However, it does not need any more adjustments once its setting parameters have been adjusted. Moreover, the method can update models by itself when novel data are collected from new operating conditions. This property means that it can keep operating for a significant length of time without human assistance.

The second limitation is the difficulty in estimating the values of the setting parameters at the starting point of our method. It is extremely difficult to estimate the threshold needed for the complexity function. Again, human assistance is absolutely necessary for the starting settings.

The two limitations described here are clear evidence of the difficulty in creating autonomous systems. It is still a challenging task to develop systems that

auto-update their setting parameters to deal with novel data. On real production lines, the integration of the tools based on this approach remains somewhat difficult.

It is important to mention that the chromosome of the GA selected uses a binary format to represent the model parameters to be optimised. Binary-coded GAs suffer from the problem of Hamming Cliffs (Gen & Cheng, 2000). An excessive number of bits sometimes need to be changed to make small changes in a parameter. This clearly reduces the efficiency of the GA. Although the performance was not perfect, we still believe that the binary-coded chromosome to be a satisfactory solution.

As Grefenstette (1986) proposed, the problem can be avoided by using gray code instead of binary. However, we decided to keep the population size at high values in our case. We consider that this suffices to reduce the disadvantages of optimising real-valued parameters using a binary-coded GA. We agree that a real-coded chromosome is more suitable for continuous search space than its binary-coded counterpart. Nevertheless, including the FS process in the optimisation process tips the balance towards the use of the binary. In contrast to earlier researches (Goldberg *et al.*, 1992), we understand the binary-coded chromosome has certain advantages when combining optimisation with GA-based FS.

Difficulties still remain in the way of dealing with noisy data. Outliers and empty values can be easily filtered, but noise is particularly challenging problem. Future work will explore the influence of the noise on training data. Noise is very difficult to remove and industrial plants are characterised by a high ratio of noise in the variables measured. It is well-known that noise drastically reduces model accuracy. It also makes it difficult to glean meaningful knowledge from the data (Yang & Wu, 2006).

The methodology was implemented using only MLP networks. There are many types of ANNs such as Bayesian networks and RBFNs, among others. As far as we know, they might be better suited to other industrial processes. For that reason, we are currently in the process of extending the proposal to create a generic tool that includes other models. The main requierement is that model complexity hast to be controlled as in SVM-based models or MLP-based EMs.

In short, we believe that the results obtained provide evidence to confirm the efficiency and reliability of this advanced methodology compared with a

standard optimisation based on GAs.

Finally, the findings in third contribution provide enough support for using EMs to predict set points for online control systems.

Industrial processes such as CHDGLs tend to generate very large, noisy DBs that always entail a loss of accuracy, wasted time and storage problems. When dealing with these problems, the scalability of models is needed to discover knowledge due to the size of these DBs (Schlang & Lang, 2001; Paliwal & Kumar, 2009). EMs have been successfully applied in many small-scale cases. As far as we know, selecting the suitable scheme for scaling up to large industrial DBs still poses a challenge (Rokach, 2010).

The comparative methodology proposed for evaluating model performance clearly has an advantage over the previous ones. It gives robust evidence on the real performance of models, which has proved crucial for identifying those models with the highest generalisation capacity but also with low computation cost. The main explanation for this improvement is the inclusion of new metrics and the repetition of the testing process (by bootstrapping with the testing data a total of $N = 10$ times).

In addition, our comparative study took a different point of view because it focused solely on three ensemble schemes and five BLs. However, we modified model parameters while those in other studies often remain unchanged. Additionally, we did not use a small dataset that was from repositories or well-known databases; instead, all our data came from the CHDGL. This source generates data with great heterogeneity, imbalance and skewness that make it more difficult to achieve an accurate prediction.

First, the results from the evaluation of single data-driven models, which are also called base learners (BLs) in ensemble learning literature, were required in order to discuss advantages and disadvantages by comparing them with the EMs proposed. These results were obtained from previous experiments carried out by Martínez-De-Pisón *et al.* (2010b). Our results using a comparative evaluation prove that EMs are better overall models because of their lower generalisation error. This is consistent with several previous papers, such as Barai & Reich (1999), Mevik & Segtnan (2004) or Siwek *et al.* (2009).

It is important to stress that our results are in a close agreement with several performance assessments of EMs reported in the literature (Breiman, 1996; Opitz & Maclin, 1999; Minowa, 2008). Although the good performance of EMs has been well reported in computer science (Hand *et al.*, 2001; Witten & Frank, 2005; Nisbet *et al.*, 2009), we believe our results show that the benefits of using EMs to deal with small datasets could be extended to complex industrial DBs..

M5P and MLP networks are two examples of unstable learning algorithms, in which small perturbations in the training dataset can cause significant changes in predictions. In 1996, Breiman showed the effectiveness of applying bagging for combining these BLs. Remarkably, M5P-based EMs performed badly in our experiments. Although this finding differs to some extent from those of Breiman (1996), it could nevertheless be argued that a good explanation of why MLP-based EMs performed better is found in Barai & Reich (1999) and corroborated by Yang *et al.* (2011).

Note that MLP-EMS have attracted the attention of many researchers in modelling. They appear to be a very promising approach for reducing the generalisation error of models. In general, these EMs are constructed by developing a number of standard ANNs for regression problems (Witten & Frank, 2005). Several studies have already provided valuable information about the potential of many ensemble schemes. Bauer & Kohavi (1999); Opitz & Maclin (1999); Galar *et al.* (2011) are examples working on classification tasks and Pardo *et al.* (2010) on regression.

What is surprising is the fact that MLP networks such as BLs were the best in all the ensemble schemes evaluated. This might be because of the well-known ability of MLP networks have to accurately predict continuous output variables. However, our results also suggest that this property is maintained using the MLP networks as BL. This matches well with previous results reported by Niu *et al.* (2011) and Yang *et al.* (2011) and also confirms the initial findings in Pardo *et al.* (2010). Another explanation may be the ability of MLP networks to perform an overall global approximation, while other models such as RBFNs are typically local approximation methods.

The MLP networks with only three neurons in the hidden layer (MLP03) and MLP-based EM (AR-MLP, BG-MLP and DG-MLP) recorded the highest generalisation capacity. The main reason is that they struck a good balance between validation and testing errors. This is because of their less complex structure, which means they are not so specialised as in previously known data. It

should be noted that some of these less comlex models sometimes even present fewer testing errors than validation ones. We assume that this happens because the validation dataset is more complex than the testing one in these cases.

Our results also show that MLP-based EMs are able to make similar predictions even in changing conditions, such as slight changes in inputs and variations in the setting parameters of models. This suggests that MLP-based EMs are more reliable than the other EMs studied.

In contrast, M5P-based EMs recorded a clear trend for overfitting. We were not successful in avoiding this problem, even when modifying the configuration parameters of the BL or the pruning conditions for the model trees. In modelling literature (Seni & Elder, 2010), M5P is considered an unstable model, and, consequently, it records very low validation errors. However, M5P as BL is clearly unsuitable for working in changing environments that generate large volumes of novel data. This phenomenon is graphically represented in the paper (Figures 5 and 7, Sanz-García *et al.*, 2013), leaving no doubt that M5P-based EMs have the lowest generalisation capacity of all the models.

The AR-SVM model and the EMs including LSMQ or LR as BLs failed to ensure enough accuracy in the prediction of temperature set points. The SVM, LR and LSMQ models are classified as stable, and they are included in the same group as k-nearest neighbour (k-NN) regressors (Breiman, 1996). As reported by Breiman (1994), the results that we have obtained indicate that any ensemble scheme using a stable algorithm is extremely accurate.

All the EMs developed seem to have recorded significant improvements in all features, but the reality is that their computation costs are always higher. The cost is sometimes even considered excessive for a prediction model that should be implemented in a real-time control system. For instance, the experiments prove that the computation costs associated with SVM-based EMs and MLP-based EMs with high numbers of neurons in the hidden layer are unreasonable. This result has further strengthened our conviction that using MLP with few neurons in the hidden layer and a low number of iterations in the learning process would be crucial for obtaining overall models (Martínez-De-Pisón *et al.*, 2010b, 2011).

Consequently, the improvement in both accuracy and generalisation capacity of EMs entails mainly extra computation time, lower intelligibility and higher complexity than single models. However, those BLs that make up EMs can be independently trained in parallel, decreasing the training time of EMs.

Further research could be conducted in at least two areas that build on the lastest methodology presented. First of all, the use of a weighted average method instead of simple average would be combine the outputs with different weights for each model developed. These weights could be calculated by some kind of regression modelling, such us partial least squares regression. In addition, another kind of dynamic ANN could be used to generate models that are less correlated and have higher variation or disparity between them. This could be effective for improving the generalisation capability and also the effectiveness of models dealing with novel data.

In short, we consider that the methodology proposed provides valuable information that directly enables to be taken regarding the most interesting model for developing a specific problem; and in our particular case study the information obtained and the direction of the results reveal trends in modelling process that could be of great help to plant engineers.

In conclusion, all these findings allowed us to suggest that the entire process of applying the methodologies proposed in this thesis could be used to extract valuable knowledge from the CHDGL database studied. While not all the results were significant in this thesis, their general direction points to the major possibilities the implementation of DM methodologies could have for assisting in the complex task of improving industrial processes.

Chapter 8

Conclusions

The methodologies proposed may be applied to CHDGLs to discover useful knowledge that helps plant engineers to improve galvanising processes. Our results reveal the huge number of unexplored possibilities that this knowledge can provide for developing models and decision support systems, among others.

This thesis was carried out with a view to improving the existing methodologies in two main aspects: finding association rules for explaining failures in the galvanising lines and developing better models for predicting CAF temperature set points in the CAF on the line.

The research presented in this thesis provides the following findings:

- A methodology based on simple pre-processing, segmentation and a search for hidden knowledge on the basis of TS that can be easily applied to the enhancement of production processes. The pre-processing and segmentation of TS linked to the use of ARM is shown to be extremely useful when searching for hidden knowledge in the data logs of industrial processes, which may help to reduce failures in production lines.

- A methodology based on data-driven methods for designing overall parsimonious models to predict CAF temperature set points. The proposed methodology makes it easier for plant engineers to deal with continuous product changes, spending less time on adjusting models and reducing downtime costs. The main advantages of this methodology are the reduced complexity of the final models, better generalisation capacity and the computation

time saved, whereby it can be incorporated it into a CAF's online control system.

- A comparative methodology for selecting better overall data-driven models to predict temperature set points for a CAF on a CHDGL. The comparative evaluation proves that the use of MLP network as BL is the best choice for generating the best-performing models, i.e. AR-MLP, BG-MLP and DG-MLP. In addition, it provides support for the final recommendations on using EMs as a regression technique. Their main advantages are high efficiency and reliability in terms of computation cost, generalisation capacity and ease for determining the best model configuration.

All in all, the methodologies described can make it easier for plant engineers to deal with continuous product changes, spending less time on adjusting the line, and reducing the time and cost of solving problems on production lines when dealing with new products.

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APPENDICES

Appendix A

Supplementary material for Publication I

A.1 Complete list of rules extracted from the CHDGL database

The outcome of the experimental work carried out in Publication I is just two knowledge rules that were considered "interesting" or "important". The rest of the rules extracted were classified as redundant and were eliminated. Also, those rules that were considered as equivalent to others were manually removed.

In addition, Table 4 in (Martínez-de Pisón *et al.*, 2012) was added with the first 20 rules obtained, showing the high number of the rules that were redundant. It was necessary to clarify the process for obtaining the rules. We thus attached Table A.1, Table A.2 and Table A.3 in this Appendix with all 64 rules obtained with a support of more than 50 %.

Table A.1: Rules extracted from the CHDGL database (part 1 of 3)

	items	support
1	{T9=}	0.897
2	{T3=Z06_TMP_BELOW}	0.769
3	{T5=TMP_P02_BELOW}	0.692
4	{T1=BATH_TMP_BELOW , T2=SPD_DEC, T3=Z06_TMP_BELOW}	0.667
5	{T1=BATH_TMP_BELOW , T3=Z06_TMP_BELOW}	0.667
6	{T1=BATH_TMP_BELOW , T2=SPD_DEC}	0.667
7	{T2=SPD_DEC, T3=Z06_TMP_BELOW}	0.667
8	{T3=Z06_TMP_BELOW, T4= TMP_P02_BELOW}	0.667
9	{T2=SPD_DEC}	0.667
10	{T1=BATH_TMP_BELOW }	0.667
11	{T1=BATH_TMP_BELOW , T2=SPD_DEC, T3=Z06_TMP_BELOW,T4=SPD_NOT_HOR , T5=TMP_P02_BELOW}	0.615
12	{T1=BATH_TMP_BELOW , T2=SPD_DEC, T3=Z06_TMP_BELOW, T4=SPD_NOT_HOR }	0.615
13	{T1=BATH_TMP_BELOW , T2=SPD_DEC, T4=SPD_NOT_HOR , T5=TMP_P02_BELOW}	0.615
14	{T1=BATH_TMP_BELOW , T3=Z06_TMP_BELOW, T4=SPD_NOT_HOR , T5=TMP_P02_BELOW}	0.615
15	{T1=BATH_TMP_BELOW , T3=Z06_TMP_BELOW, T4=SPD_NOT_HOR }	0.615
16	{T1=BATH_TMP_BELOW , T4=SPD_NOT_HOR , T5=TMP_P02_BELOW}	0.615
17	{T1=BATH_TMP_BELOW , T2=SPD_DEC, T4=SPD_NOT_HOR }	0.615
18	{T2=SPD_DEC, T3=Z06_TMP_BELOW, T4=SPD_NOT_HOR , T5=TMP_P02_BELOW}	0.615
19	{T2=SPD_DEC, T3=Z06_TMP_BELOW, T4=SPD_NOT_HOR }	0.615
20	{T2=SPD_DEC, T4=SPD_NOT_HOR , T5=TMP_P02_BELOW}	0.615
21	{T3=Z06_TMP_BELOW, T4=SPD_NOT_HOR , T5=TMP_P02_BELOW}	0.615
22	{T3=Z06_TMP_BELOW, T4=SPD_NOT_HOR }	0.615
23	{T4=SPD_NOT_HOR , T5=TMP_P02_BELOW}	0.615

Table A.2: Rules extracted from the CHDGL database (part 2 of 3)

	items	support
24	{T2=SPD_DEC, T4=SPD_NOT_HOR }	0.615
25	{T1=BATH_TMP_BELOW , T4=SPD_NOT_HOR }	0.615
26	{T1=BATH_TMP_BELOW , T2=SPD_DEC, T3=Z06_TMP_BELOW, T5=TMP_P02_BELOW}	0.615
27	{T1=BATH_TMP_BELOW , T2=SPD_DEC, T5=TMP_P02_BELOW}	0.615
28	{T1=BATH_TMP_BELOW , T3=Z06_TMP_BELOW, T5=TMP_P02_BELOW}	0.615
29	{T1=BATH_TMP_BELOW , T5=TMP_P02_BELOW}	0.615
30	{T2=SPD_DEC, T3=Z06_TMP_BELOW, T5=TMP_P02_BELOW}	0.615
31	{T2=SPD_DEC, T5=TMP_P02_BELOW}	0.615
32	{T3=Z06_TMP_BELOW, T5=TMP_P02_BELOW}	0.615
33	{T4=SPD_NOT_HOR }	0.615
34	{T5=TMP_P02_BELOW, T9=}	0.589
35	{T1=BATH_TMP_BELOW , T2=SPD_DEC, T3=Z06_TMP_BELOW, T9=}	0.564
36	{T1=BATH_TMP_BELOW , T2=SPD_DEC, T9=}	0.564
37	{T1=BATH_TMP_BELOW , T3=Z06_TMP_BELOW, T9=}	0.564
38	{T1=BATH_TMP_BELOW , T9=}	0.564
39	{T2=SPD_DEC, T3=Z06_TMP_BELOW, T9=}	0.564
40	{T2=SPD_DEC, T9=}	0.564
41	{T8=, T9=}	0.538
42	{T8=}	0.538
43	{T1=BATH_TMP_BELOW , T2=SPD_DEC, T3=Z06_TMP_BELOW, T4=SPD_NOT_HOR , T5=TMP_P02_BELOW, T9=}	0.513
44	{T1=BATH_TMP_BELOW , T2=SPD_DEC, T4=SPD_NOT_HOR , T5=TMP_P02_BELOW, T9=}	0.513
45	{T1=BATH_TMP_BELOW , T2=SPD_DEC, T3=Z06_TMP_BELOW, T4=SPD_NOT_HOR , T9=}	0.513
46	{T1=BATH_TMP_BELOW , T2=SPD_DEC, T4=SPD_NOT_HOR , T9=}	0.513

Table A.3: Rules extracted from the CHDGL database (part 3 of 3)

	items	support
47	{T1=BATH_TMP_BELOW , T3=Z06_TMP_BELOW, T4=SPD_NOT_HOR , T5=TMP_P02_BELOW, T9=}	0.513
48	{T1=BATH_TMP_BELOW , T4=SPD_NOT_HOR , T5=TMP_P02_BELOW, T9=}	0.513
49	{T1=BATH_TMP_BELOW , T3=Z06_TMP_BELOW, T4=SPD_NOT_HOR , T9=}	0.513
50	{T1=BATH_TMP_BELOW , T4=SPD_NOT_HOR , T9=}	0.513
51	{T2=SPD_DEC, T3=Z06_TMP_BELOW, T4=SPD_NOT_HOR , T5=TMP_P02_BELOW, T9=}	0.513
52	{T2=SPD_DEC, T4=SPD_NOT_HOR , T5=TMP_P02_BELOW, T9=}	0.513
53	{T2=SPD_DEC, T3=Z06_TMP_BELOW, T4=SPD_NOT_HOR , T9=}	0.513
54	{T2=SPD_DEC, T4=SPD_NOT_HOR , T9=}	0.513
55	{T3=Z06_TMP_BELOW, T4=SPD_NOT_HOR , T5=TMP_P02_BELOW, T9=}	0.513
56	{T4=SPD_NOT_HOR , T5=TMP_P02_BELOW, T9=}	0.513
57	{T3=Z06_TMP_BELOW, T4=SPD_NOT_HOR , T9=}	0.513
58	{T4=SPD_NOT_HOR , T9=}	0.513
59	{T1=BATH_TMP_BELOW , T2=SPD_DEC, T3=Z06_TMP_BELOW, T5=TMP_P02_BELOW, T9=}	0.513
60	{T1=BATH_TMP_BELOW , T2=SPD_DEC, T5=TMP_P02_BELOW, T9=}	0.513
61	{T1=BATH_TMP_BELOW , T3=Z06_TMP_BELOW, T5=TMP_P02_BELOW, T9=}	0.513
62	{T1=BATH_TMP_BELOW , T5=TMP_P02_BELOW, T9=}	0.513
63	{T2=SPD_DEC, T3=Z06_TMP_BELOW, T5=TMP_P02_BELOW, T9=}	0.513
64	{T2=SPD_DEC, T5=TMP_P02_BELOW, T9=}	0.513

Appendix B

Supplementary material for Publication II

B.1 Evolution of the attribute selection in THC3 and THC5 prediction models

The behaviour of the GAs selection carried out in the experiments for predicting temperature THC1 was included in the paper as Figure 16 in (Sanz-García *et al.*, 2012). The rest of the experimental results obtained during *THC3* and *THC5* models´ optimisation was uploaded as Supplementary Material. For that reason, processes of attribute selection for *THC3* and *THC5* prediction models are included as Figure B.1 and Figure B.2, showing the percentage of ten best models that included the input (vertical axis) via the number of generation (horizontal axis).

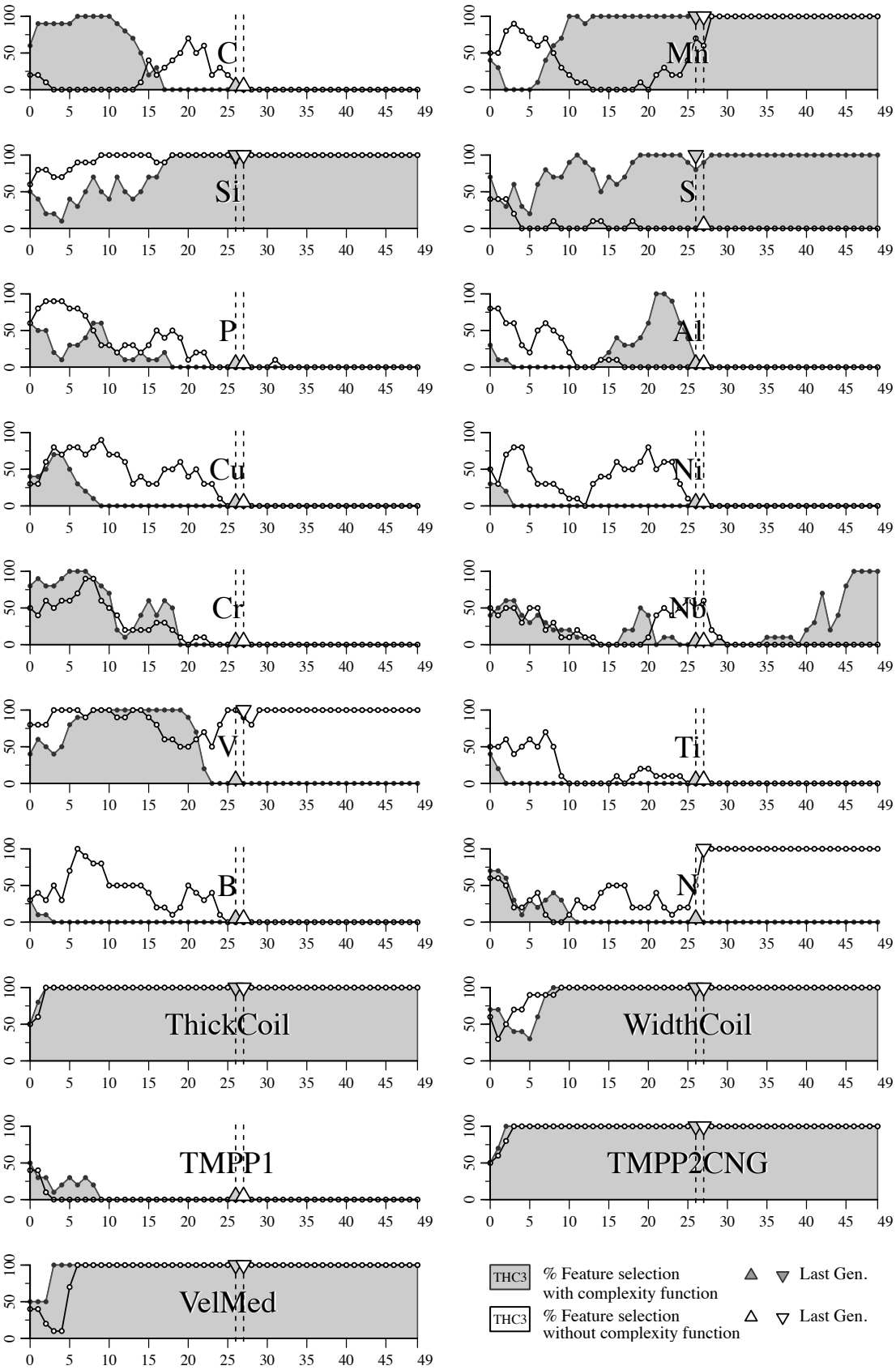

Figure B.1: Evolution of attribute selection for all inputs in THC3 *models*

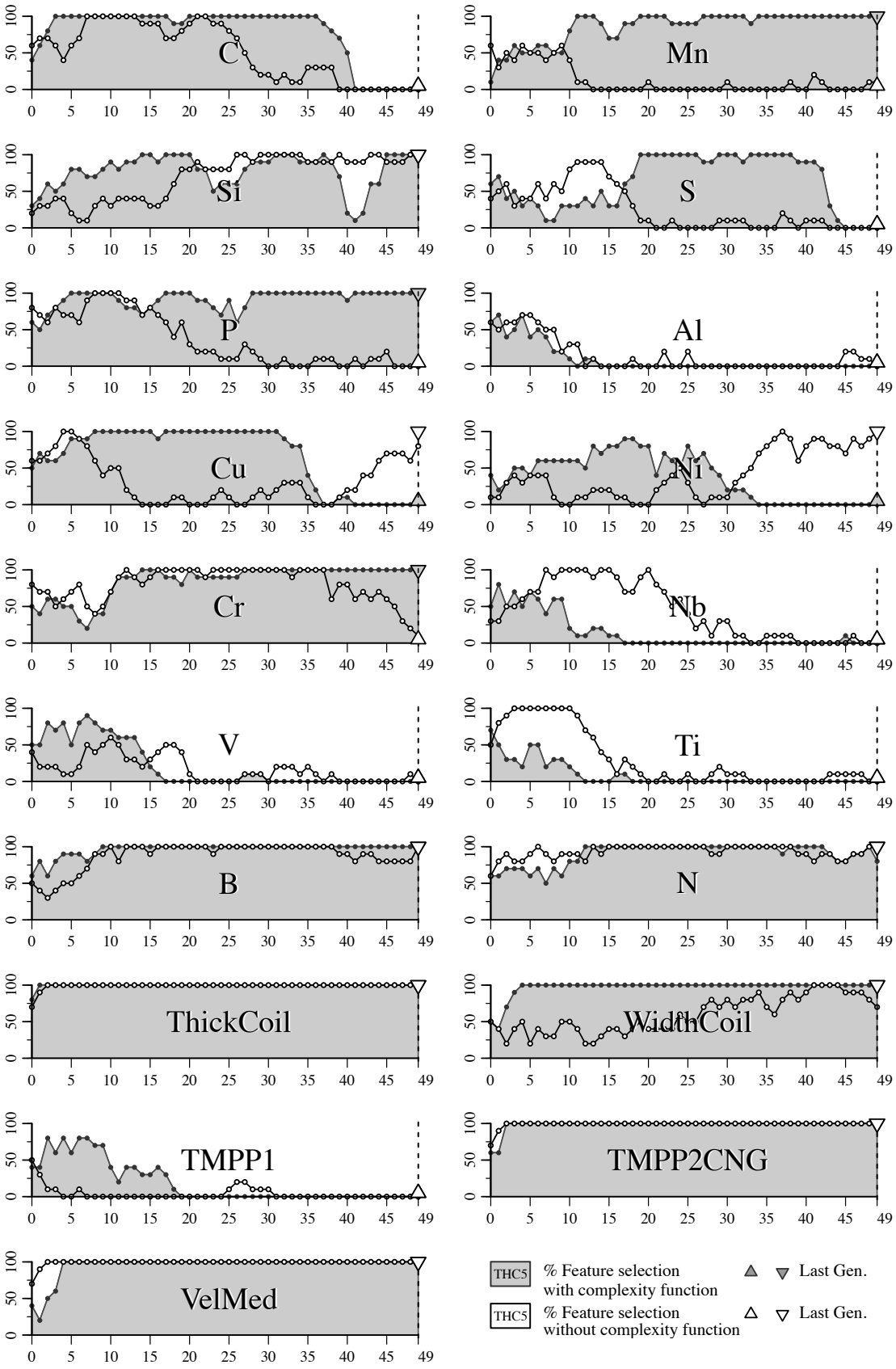

Figure B.2: Evolution of attribute selection for all inputs in THC5 *models*

B.2 Figures for evaluating aggregation coefficients W

Figure 15 in (Sanz-García *et al.*, 2012) shows the representation of validation and testing $RMSE$ via aggregation coefficient W for MLP networks developed during 50 generations. The range of the aggregation coefficients was cut at value $W = 15$. The full range provides more information about the distribution of the different values of complexity for all generations. Figure B.3, Figure B.4 and Figure B.5 show the $RMSE$ values via processes aggregation coefficients W for temperature *THC1*, *THC3* and *THC5* respectively. Black points represent validation and grey points are testing data. The results of the prediction models developed with complexity control are on the left side and without on the right side.

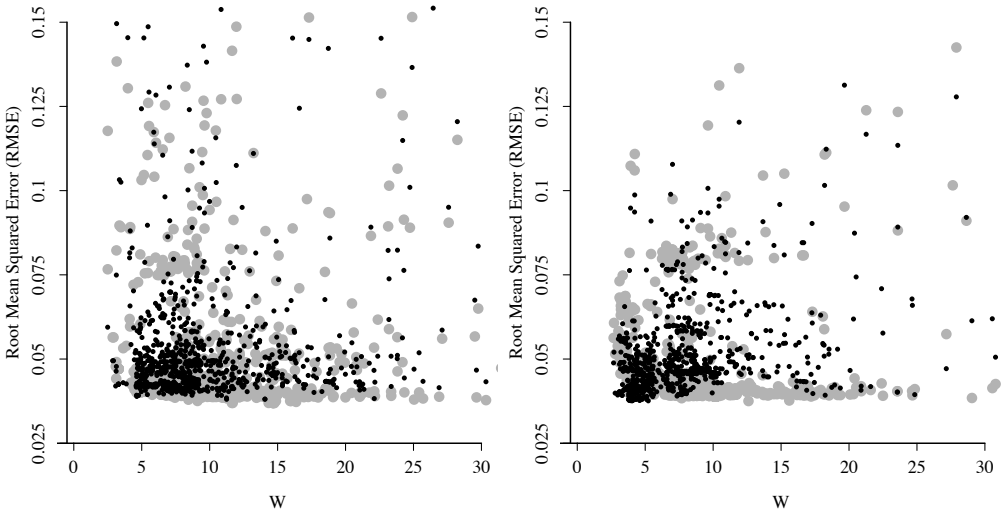

Figure B.3: Complete range of $RMSE$ via aggregation coefficients W: THC1

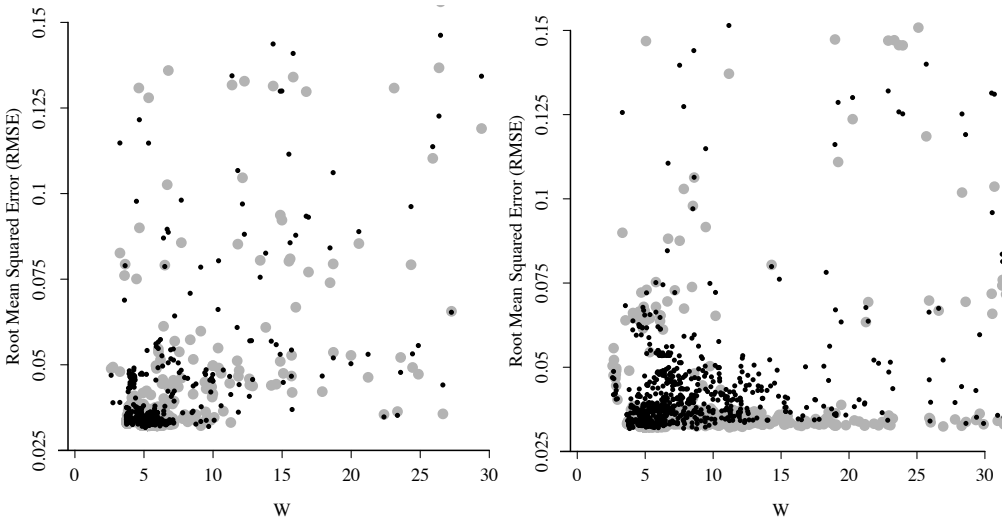

Figure B.4: Complete range of $RMSE$ via aggregation coefficients W: THC3

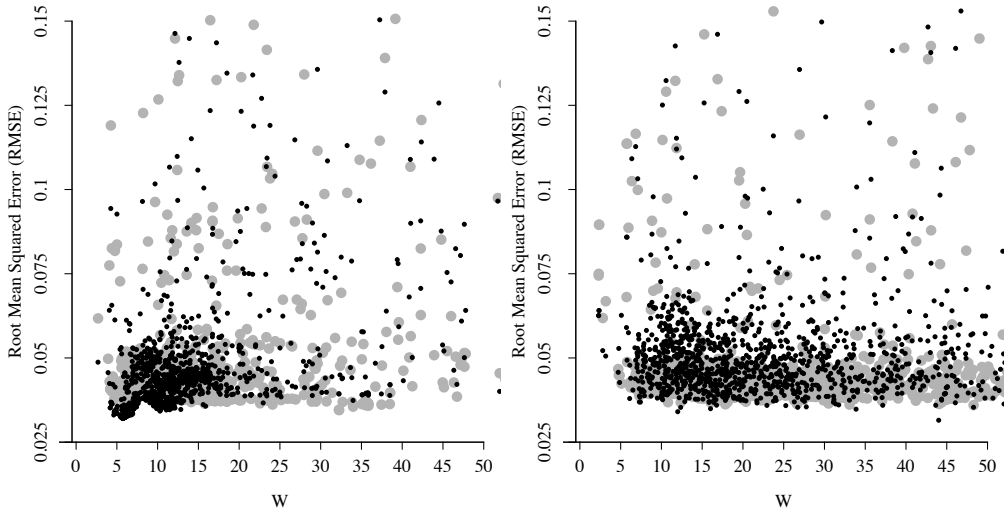

Figure B.5: Complete range of $RMSE$ via aggregation coefficients W: THC5