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RESEARCH

Machine Learning Approaches to Predict the Hardness of Cast Iron

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A B S T R A C T

The accurate prediction of the mechanical properties of foundry alloys is a rather complex task given the substantial variability of metallurgical conditions that can be created during casting even in the presence of minimal variations in the constituents and in the process parameters. In this study an application of different intelligent methods of classification, based on the machine learning, to the estimation of the hardness of a traditional spheroidal cast iron and of a less common compact graphite cast iron is proposed. Microstructures are used as inputs to train the neural networks, while hardness is obtained as outputs. As general result, it is possible to admit that 'light' open source self-learning algorithms, combined with databases consisting of about 20-30 measures are already able to predict hardness properties with errors below 15 %.

1. INTRODUCTION

The cast iron consists of a large family of iron-carbon alloys where the presence of carbon is greater than 2 % in weight [1,2]. According to the chemical composition and process parameters, each alloy can be characterized by a specific microstructure, mechanical properties, tribology and, ultimately, a specific practical use [3].

Few changes in chemical balances (as additives inoculation [4]) or in the metallurgical conditions are sufficient to produce materials with very different characteristics and applications [5,6], from the common gray iron to the high performing ductile cast iron [7,8].

Thanks to this flexibility, cast iron represents one of the most appreciate materials, with a relevant role in the mankind history as in the present [9].

The first attempts at producing cast iron in the Mediterranean basin can be traced back to over 1000 BC while the earliest artifacts, date to the 5th century BC, were found in China [9]. Tower ovens, essential to allow the metal to gain the right temperature, were found in Sweden, dated between 1150 and 1350, while the beginning of

Renaissance also reported the first cannons made of cast irons [9].

From the other side, this versatility is paid with the difficulty to predict the material properties. This consideration is also true in the case of the surface hardness, where, the overall variability of the material can be aggravated by additional aspects, related to local effects [10].

However, respect to an industrial interest, it is often enough to have quick indications on these material properties, even not extremely precise. In this study the application of the concepts of Artificial Intelligence (AI) and Machine Learning (ML) [11] are proposed to estimate the hardness of a spheroidal iron (SGI) [12,13] and a less common compact graphite iron (CGI) [13-15].

Microstructural macro-indicators, as, e.g., the quantity of graphite, ferrite, perlite in the alloy, acquired by microstructures, are used as inputs to train three (3) different AI algorithms, while hardness properties are obtained as outputs.

Two datasets of measures from tests were considered, one per each material, consisting of 20-30 samples, while comparisons of predictions were done by a direct correlations.

2. MACHINE LEARNING

The Machine Learning (ML) is a branch of the Artificial Intelligence (AI) that collects a set of methods, developed from the last decades of the 20th century in various scientific communities, under different names [16] as: computational statistics, pattern recognition, artificial neural networks, adaptive filtering, theory of dynamic systems, data mining, adaptive algorithms and so on. It uses statistical methods to progressively improve the performance of an algorithm in identifying patterns inside the available data.

The same Arthur Samuel who coined the term of Machine Learning in 1959 [17] identifies in terms of principles two distinct approaches.

The first method [18], referred to as an Artificial Neural Network (ANN), leads to the development of general-purpose ML machines in which the 'behavior' is learned from a randomly connected switching network, following a learning routine based on the concept of reward and punishment (reinforcement learning). The process of determining the values of these connections on the basis of a data set is referred to as training or training, and therefore the data set is usually referred to as a training set [19].

The second one [18], more specific, reproduces the equivalent of a highly organized network, designed to learn only certain specific activities. Using a supervision, this procedure requires a new programming for each new application, but appears to be much more efficient from a computational point of view.

Independently by the approach, the ML is closely linked to pattern recognition and to the computational theory of learning [18], while explores the study and construction of algorithms that can learn from a set of data and make predictions about them, building into inductive way a model based on samples. Thus, ML can be particularly appreciate in those fields in which decisions and predictions cannot be related to the use of explicit logics. In industry its applications are strongly related to the solution of engineering problems, based on mathematical optimization and evaluations.

In these terms, the process of learning is based on a phase when the pattern recognition is implemented by a classifier able to track down features and weights from data, also benefitting by probabilistic approaches.

A large choice of models and algorithms have been developed in the years [20]. Between many others, the following ones were preferred in this investigation in consideration of valid results emerged in previous similar researches [21].

2.1 Random Forest (RF)

The RF is one of the most popular and effective methods for solving the problems in ML, such as classification and regression [22]. In appearance, the learning algorithm is rather simple (especially when compared with the learning algorithm of other methods). The basic ideas laid down in binary decision tree, bootstrapping aggregation or bagging, random subspace method and decorrelation.

2.2 Neural Network (NN)

NNs offer a very powerful and general structure for representing a non-linear mapping of several input variables for several output variables [23]. A NN is a structure (network) consisting of a set of interconnected links (artificial neurons). Each link has a characteristic value for input and output and implements a local calculation or function. The output of any link is determined by the characteristics of its input and output, its relationship with other links, as well as external inputs, if any. Besides, the NN topology is an important issue, since the overall applicability of the NN to the specific problem depends on it. A multi-layered topology is commonly adopted.

2.3 k-nearest neighbors (kNN)

The kNN is a non-parametric method used for classification and regression [24]. The input consists of the k closest training examples in the feature space. The output depends on whether k-NN is used for classification or regression.

In the case of classification, the output is a class membership. An object is classified by a plurality vote of its neighbors, with the object being assigned to the class most common among its k nearest neighbors (k is a positive and small integer). In the case of regression, the output is the property value for the object. This value is the average of the values of its k nearest neighbors. In any case, the k-NN can be considered as a type of instance-based learning, or lazy learning, where the function is only approximated locally and the computation is deferred until classification. The k-NN algorithm is among the simplest of all ML algorithms. A peculiarity of the k-NN algorithm is that it is sensitive to the local structure of the data.

3. DATA MINING

Measures for ML of algorithms derived from experiments already discussed in details in previous works [25-28]. In particular, they describe a large experimental experience that permitted to characterize material samples in SGI and CGI coming from 4 metal castings, implemented in two different days. Special care was taken to assure similar conditions of casting in terms of chemical composition, temperature and other process parameters [29].

For instance, those castings used for extracting samples for testing, were realized after several hours of foundry production in the way to stabilize temperature and metallurgy. Moreover, chemical composition tests, performed during production, permitted to verify the consistency and stability of melt alloy (Fig. 1).

a) b) c)

Fig. 1. Different phases of chemical inspection during the processing: a) molten metal extraction; b) manual transport; c) spilling on the instrument for the detection of chemical elements.

Entering in further details, in accordance with [28] the measures under consideration belong to 27 samples in SGI and 21 samples in CGI.

As input for ML, the following metallographic parameters were chosen:

- Quantity of Graphite
- Quantity of Ferrite
- Quantity of Perlite
- Grade of Nodularity
- Grade of Vermicularity

with values expressed in percentage.

These data, expressed in percentages (%), were provided in terms of single values estimated by considerations on micrographs (as in Fig. 2).

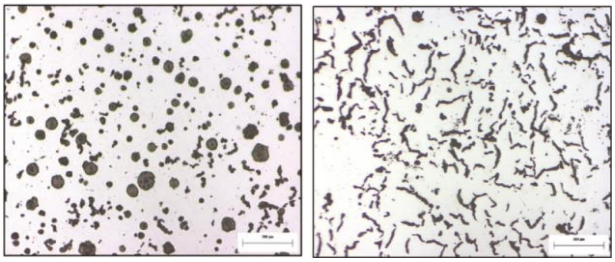

Fig. 2. Example of micrographs (100x) with different grade of vermicularity: from their image analysis metallographic parameters were evaluated.

Using an image analysis software, the geometric parameters related to graphite (area, perimeter, diameter of Feret, etc.) were acquire by micrograph. Each sample (in SGI or CGI) provided a specific set of 5 (five) values, as reported in Tables 1 and 2. Every set (in total 27+21) of metallographic characteristics was combined with the related hardness property, as measured by Brinell test (HB).

Table 1. Metallographic properties of SGI.

N.	Graphite	Ferrite	Perlite	Nodu Larity	Vermi cularity
1	13.6	42.5	43.9	75.2	17.0
2	6.3	52.8	40.9	56.4	34.4
3	10.2	55.7	34.1	77.7	16.6
4	12.1	48.5	39.5	67.1	26.2
5	11.2	42.8	46.0	68.8	23.7
6	12.2	47.1	40.8	63.6	27.2
7	8.6	48.6	42.8	62.6	30.4
8	9.1	47.5	43.4	53.9	36.8
9	12.6	43.6	43.8	79.0	15.2
10	7.0	51.6	41.4	72.5	19.7
11	13.7	39.2	47.1	84.4	10.8
12	8.1	49.0	42.9	75.7	17.3
13	7.1	45.2	47.7	61.9	27.6
14	7.6	33.5	58.8	84.6	10.2
15	7.1	44.6	48.3	68.6	22.3
16	9.4	47.3	43.4	75.1	17.1
17	8.3	43.6	48.1	50.9	40.9
18	8.6	43.7	47.8	65.7	24.3
19	12.1	44.8	43.1	75.5	17.1
20	11.3	30.5	58.2	85.7	9.4
21	13.2	34.2	52.7	86.1	9.4
22	9.2	40.8	50.0	66.9	23.6
23	9.1	32.1	58.8	78.2	16.3
24	10.2	30.8	59.1	80.8	14.1
25	7.0	22.7	70.3	81.6	11.9
26	9.3	24.6	66.1	89.6	5.9
27	6.5	24.8	68.7	74.2	17.7
μ	9.7	41.2	49.2	72.7	20.1
σ	2.3	9.0	9.4	10.2	8.8
σ%	24	22	19	14	44

Table 2. Metallographic properties of SGI.

N.	Graphite	Ferrite	Perlite	Nodu larity	Vermi Cularity
1	16.7	53.5	29.8	9.0	88.9
2	21.0	60.2	18.8	16.1	81.2
3	12.6	61.9	25.6	11.7	86.4
4	17.3	62.3	20.4	12.1	85.1
5	15.7	64.3	20.0	17.5	79.7
6	13.9	62.9	23.2	15.4	82.2
7	11.2	65.8	22.9	17.9	80.0
8	14.5	62.6	22.9	23.4	74.3
9	13.2	64.8	22.0	13.0	84.4
10	14.5	61.6	23.9	9.4	88.5
11	14.6	56.6	28.9	19.5	78.5
12	10.3	63.0	26.8	16.7	81.4
13	10.1	62.9	27.0	16.7	81.7
14	9.7	55.2	35.2	13.3	85.4
15	12.6	53.4	34.0	16.3	81.9
16	12.8	58.3	28.9	24.0	74.0
17	11.1	63.5	25.5	16.2	81.8
18	12.9	52.9	34.2	18.5	79.5
19	11.4	64.9	23.7	15.1	82.7
20	9.8	59.9	30.3	17.8	80.5
21	9.2	67.6	23.3	21.6	74.6
μ	13.0	61.2	25.8	16.6	81.2
σ	3.0	4.3	4.7	4.0	4.2
σ%	23	7	18	24	5

Focusing the attention on these parameters, it is evident a not marginal variability in their values. The relative standard deviation ($\sigma_{\%}$), expressed as the ratio between the standard deviation (σ), and the mean value (μ) permits a homogeneous comparison. In particular, in the case of SGI, the variability of the metallographic factors under investigation, expressed by $\sigma_{\%}$, is between 14 % (nodularity) and 44 % (vermicularity). This variability is lower in the case of CGI, between 5 % (vermicularity) and 24 % (nodularity).

The difficulty in using this kind of information for performing valid predictions on material properties is evident in Table 3 where the correlation between parameters is estimated by the Pearson correlation coefficient (considering all properties, including the Brinel hardness, and both alloys). It is largely known that this coefficient ($\boldsymbol{\rho_{xy}}$) is able to measure the linear correlation between two variables: 0 is no linear correlation, and −1 is total negative linear correlation (Fig. 3).

According to the Cauchy–Schwarz inequality it has a value between +1 and −1, where 1 is total positive. Values in the middle are typical of intermediate dependencies.

Table 3. Correlation between parameters.

SGI	Graphite	Ferrite	Perlite	Nodul.	Vermic.	HB	CGS
Graphite	1.00	-0.20	-0.45	-0.24	0.20	-0.74	Graphite
Ferrite	0.04	1.00	-0.79	0.13	-0.19	0.14	Ferrite
Perlite	-0.29	-0.79	1.00	0.03	0.05	0.33	Perlite
Nodul.	0.34	0.13	0.03	1.00	-0.99	0.54	Nodul.
Vermic.	-0.30	-0.19	0.05	-0.99	1.00	-0.52	Vermic.
HB	-0.35	0.14	0.33	0.54	-0.52	1.00	HB
SGI	Graphite	Ferrite	Perlite	Nodul.	Vermic.	HB	CGS

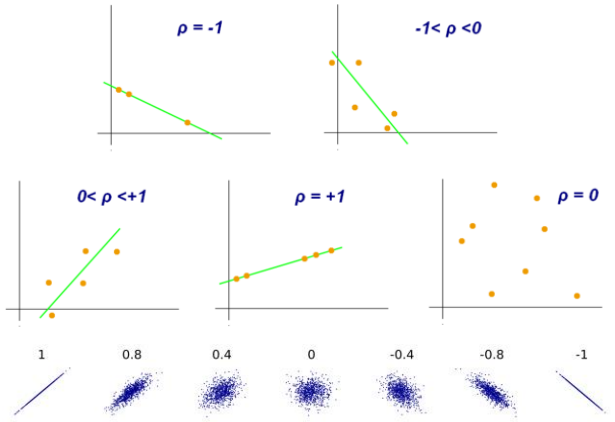

Fig. 3. Examples of scatter diagrams with different values of correlation coefficient (ρ_{xy}).

In particular, by Table 3 it can be observed, as was also expected in consideration of the way to define these parameters, a perfect negative correlation between nodulary and vermicularity ($\rho_{xy} = -1$).

Furthermore, both metallographic properties act discreetly influencing the surface hardness (approx. ±0.5). Regarding the other parameters, the analysis highlights, for both SGI and CGI, inverse correlations between:

- perlite and ferrite (strong)
- perlite and graphite (low/medium)
- ferrite and graphite (low/medium).

These correlations can be easily traced back in literature [30,31], but they are here presented to show how several aspects can simultaneously impact in the definition of the material properties. These parameters, as said, represent the multifaceted input of the ML algorithms.

Focusing now the attention on the material output, thanks to the Table 3 a general dependency can be detected for the hardness: apart for the already mentioned dependency respect to the nodulary and vermicularity, also the graphite shows its (inverse) influence on the hardness, especially in the case of SGI (=-0.74).

At the same time, the table gives evidence of the complexity behind these relations.

In other terms, Tables 1 and 2 demonstrate that experimental data are commonly affected by an not-negligible inaccuracy while Table 3 highlights that correlations between properties exist but are, in part, hidden under several mutual influences [32].

4. DATA ESTIMATIONS

This situation can be conveniently faced up by AI and ML systems. In particular, their algorithms can be shown properly adequate to find deep relationships between the available data, not directly evident, thanks to the construction of interconnection networks placed on various levels of analysis.

For the same reason, they can also prove particularly robust with respect to the use of data affected by intrinsic variability.

Evaluations on data were implemented by Orange software code, an open source ML and data visualization system [33]. Its ANNs were learned by these measures and provided outputs in terms of Brinell hardness (HB).

Specifically, per each sample, the code provided 3 (three) different estimations of hardness in accordance with the 3 (three) specific methods used:

- Random Forest (RF)
- Neural Network (NN)
- k-Nearest Neighbors (kNN)

Table 4 reports the specific parameters selected in training the ML algorithms.

Table 4. Parameters in Machine Learning.

Random Forest (RF)	
Number of trees	15
Fixed seed for random generator	32
Do not split subset smaller than	5

Neural Network (NN)	
Learning speed	0.6
Inertial coefficient	0.5
Test mass tolerance	0.02
Tolerance of the learning set	0.03
Number of layers	5

k-Nearest Neighbors (kNN)	
Metric	Chebyshev
Number of neighbour	2
Weight	Uniform

Results are reported in Tables 5 and 6, together with the related values of:

- mean value (**μ**),
- standard deviation (**σ**),
- relative standard deviation (**σ%**),
- Pearson correlation coefficient (**ρxy**).

in the way to show the overall variability of values and permit a comparison of methods.

5. RESULTS

Measures and estimations can be graphically observed and compared in Fig. 4 in both cases: SGI and CGI. In particular, in that figure, the estimation provided by (only) the *NN* method was reported since, according to the Pearson correlation coefficients (ρ_{xy}) of Tables 5 and 6, the *NN* can be considered the most appropriate method for the evaluation. In fact, with values of 0.59 and 0.43 in the case of, respectively, CGI and SGI, the *NN* demonstrates a good (even not perfect) correlation between the experimental dataset and the estimated hardness.

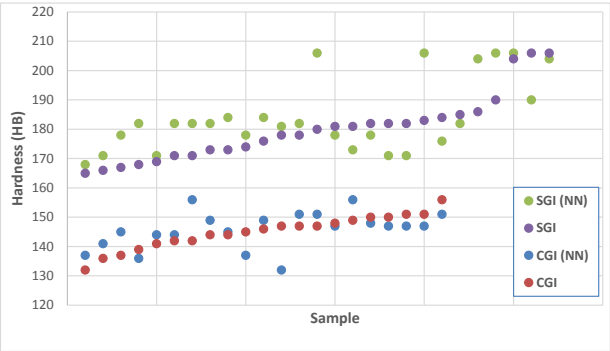

Fig. 4. Measured and estimated hardness (HB) for SGI and CGI.

This estimation is able to guarantee a substantial coincidence on the average values of hardness (184 vs 180 in the case of SGI, 146 vs 144 for CGI) and its variability (e.g. in terms of relative standard deviations). It means that, as shown in Fig. 5, there is a significant overlapping between the density functions, when measures and estimations are represented in terms of probability distributions.

Table 5. SGI Hardness as measured and estimated.

N.	HB	RF	NN	kNN
1	165	182	168	181
2	166	174	171	171
3	167	178	178	173
4	168	182	182	169
5	169	182	171	168
6	171	182	182	169
7	171	182	182	166
8	173	171	182	171
9	173	182	184	165
10	174	181	178	167
11	176	204	184	165
12	178	182	181	165
13	178	181	182	171
14	180	176	206	183
15	181	178	178	169
16	181	173	173	165
17	182	178	178	171
18	182	173	171	165
19	182	178	171	171
20	183	184	206	180
21	184	180	176	176
22	185	169	182	169
23	186	190	204	180
24	190	185	206	180
25	204	206	206	206
26	206	183	190	180
27	206	204	204	180
μ	180	182	184	173
σ	11	9	12	9
σ%	6%	5%	7%	5%
ρxy	1.00	0.48	0.61	0.58

Table 6. CGI Hardness as measured and estimated.

N.	HB	RF	NN	kNN
1	132	148	137	137
2	136	141	141	139
3	137	145	145	142
4	139	142	136	136
5	141	142	144	142
6	142	147	144	141
7	142	151	156	147
8	144	142	149	141
9	144	142	145	137
10	145	132	137	137
11	146	150	149	147
12	147	147	132	132
13	147	147	151	151
14	147	147	151	151
15	148	150	147	132
16	149	147	156	144
17	150	146	148	146
18	150	142	147	142
19	151	147	147	147
20	151	147	147	147
21	156	147	151	141
μ	145	145	146	142
σ	6	4	6	6
σ%	4%	3%	4%	4%
ρxy	1	0.17	0.46	0.30

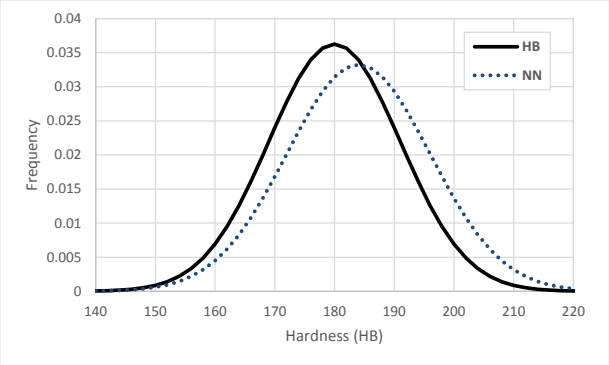

Fig. 5. Overlapping in the density function between measures and estimations (in the case of SGI and NN).

Moreover, all ANN methods under investigation seem able to provide an adequate estimation. This aspect is displayed in Fig. 6 where values from the different methods (MF, NN and kNN) are shown in the case, for instance, of SGI. The influence of the method in the estimation is marginal when compared to the general variability of measures. In particular, in the graph it is possible to see how the variability in hardness predictions was limited within a range of 30-34 % respect to the average measure.

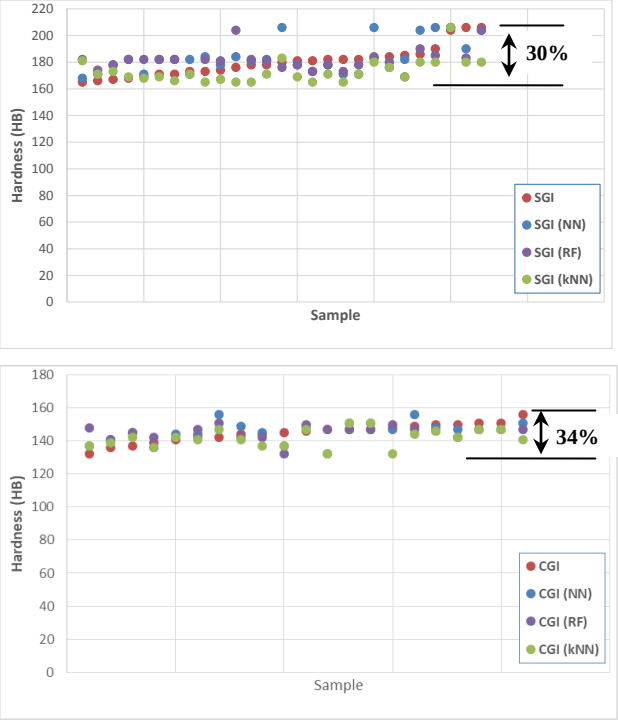

Fig. 6. Comparison between the estimation methods in the case of SGI and CGI.

This result can be considered more than appropriate concerning that:

- even if the specimens were extracted from similar casting conditions, the experimental values were characterized by a certain intrinsic variability (σ = 11). This variability was transferred through the ML process even if it is also evident a tendency toward an overall reduction.
- ML algorithms have not been optimized, nor as structure or training. This choice is related to an investigation strategy aiming at demonstrating their general applicability, without entering in specific details on AI methods.

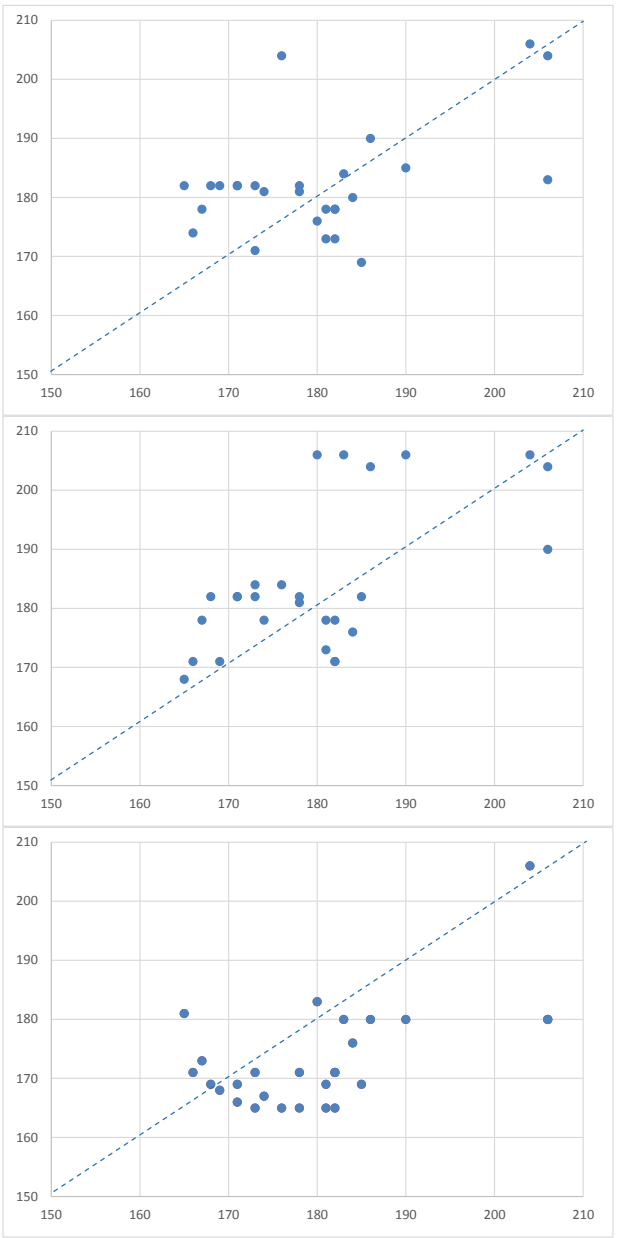

Fig. 7. Correlation between measures (x-axis) and estimations (y-axis) as predicted by RF, NN, kNN methods (in the case of SGI).

Figure 7 shows, point by point, the correlation between measures and estimations as

predicted by RF, NN, kNN (in the case of SGI). It shows, ultimately, the capability of the ML approach to find correlation in the experimental data. The grouping of values around the diagonal shows this good match. But they also show that the values that deviate greatly from this linearity are very few. Moreover, the fact that the points are distributed above and below the line lets us imagine the non-existence of systematic errors in the estimate.

6. CONCLUSION

The present research deals with the use of artificial intelligent (AI) methods in prediction of hardness of spheroidal cast iron (SGI) and compact graphite cast iron (CGI). Results from previous experiments were used to train three ANNs, based on three different principles. Open source and easy accessible algorithms were used. Even if in the presence of a limited number of measures, the ML approach, independently of the specific network, is able to predict the hardness with an acceptable confidence (±15 %).

It is also believed that a greater accuracy could be easily achieved by: i) increasing the sample of measures on which the ML code is trained; ii) optimizing the ML code in terms of depth and quality of analysis ('deep learning'), but also preferring other methods (e.g. Multiple Regression, Genetic Programming, Support Vector Machine…); iii) using microstructural information directly at a level of details, as done by the largest part of available researches.

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Nomenclature

SGI	-	Spheroidal (nodular) cast iron
CGI	-	Compact graphite cast iron
HB	-	Brinell hardness
AI	-	Artificial Intelligence
ANNs	-	Artificial Neural Networks
ML	-	Machine Learning
RF	-	Random Forest method
NN	-	Neural Network method
kNN	-	k-Nearest Neighbors method
μ	-	Mean Value
σ	-	Standard Deviation
$\sigma_{\%}$	-	Relative Standard Deviation
ρ_{xy}	-	Pearson Correlation Coefficient