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Machine Learning Prediction of Mechanical and Durability Properties of Recycled Aggregates Concrete

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Abstract

Whilst recycled aggregate (RA) can alleviate the environmental footprint of concrete production and the landfilling of colossal amounts of demolition waste, there is need for robust predictive tools for its effects on mechanical and durability properties. In this thesis, state-of-the-art machine learning (ML) models were deployed to predict properties of recycled aggregate concrete (RAC). A systematic review was performed to analyze pertinent ML techniques previously applied in the concrete technology field. Accordingly, three different ML methods were selected to determine the compressive strength of RAC and perform mixture proportioning optimization. Furthermore, a gradient boosting regression tree was used to study the effects of RA and several types of binders on the carbonation depth of RAC. The ML models developed in this study demonstrated robust performance to predict diverse properties of RAC.

Keywords

Machine learning; Recycled aggregate concrete; Mixture proportioning; Compressive strength; Carbonation depth; Durability; Gradient boosting regressor; Deep learning; Supplementary cementitious materials.

Summary for Lay Audience

Worldwide concerns regarding the environmental footprint of concrete production have imposed more rigorous requirements for construction and urban development. To enhance the sustainability of concrete, it is important to enhance its durability, lower the energy consumption in its production and placement processes, and promote the use of recycled materials in its mixture design. In the pursuit of such goals, this study explores the mechanical and durability properties of recycled aggregate concrete.

Recycled aggregate concrete (RAC) could contribute to mitigating the local shortages of natural aggregates, prevent the landfilling of massive amounts of construction and demolition waste, and reduce carbon emissions of concrete construction. Accordingly, this thesis presents state-of-the-art machine learning (ML) models to predict two main properties of RAC: compressive strength and resistance to carbonation. The development of these ML models ensured that the used datasets were diverse and comprehensive to capture the intrinsic principles involved in the properties of RAC. The carbonation depth of RAC was predicted for the first-time using ML. Furthermore, a hybrid ML model was developed to optimize the mixture design of RAC for various classes of compressive strength. The results demonstrated the superiority of ML techniques in the prediction of RAC properties. The models developed herein could be further harvested to achieve sustainable production of concrete with optimal recycled aggregate content, least cost, higher durability, and least environmental footprint.

Co-Authorship Statement

The present thesis has been structured according to the regulation of integrated-article format stipulated by the School of Graduate and Postdoctoral Studies (SGPS) at Western University. The second, third, and fourth chapters have been submitted for publication to peer-reviewed journals. All data analysis and writing were carried out by the candidate under the guidance and supervision of Professor Moncef L. Nehdi. Any other co-author contributed in the edition, and general development of the final versions of the submissions.

Itzel Nunez, Afshin Marani, Majdi Flah and Moncef L. Nehdi. Machine Learning Prediction of Compressive Strength of Modern Concrete: Systematic Review. Manuscript submitted for publication.

Itzel Nunez, Afshin Marani, Moncef L. Nehdi. Mixture Optimization of Recycled Aggregate Concrete Using Hybrid Machine Learning Model. *Materials*, MDPI, 13(4331), 1-24

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Dedication

With love to Rodrigo,

Oliva, Doly, Emma, Humberto,

Luis, Ivonne, Jesús, and Luis.

Gracias.

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Chapter 1

1 Introduction

Concrete is the second world's most consumed material, just after water. The versatility of concrete has prompted its utilization resulting in uncountable concrete structures worldwide. However, the ever-increasing urbanization has led to unsustainable growth of the concrete industry associated with several environmental issues. The construction industry is a primary consumer of natural resources, thus, several places over the world are experiencing shortages of natural aggregate (Duan *et al.*, 2013). It is estimated that the consumption of natural aggregates will continue growing such that by 2022 it will reach 66.3 billion tons worldwide (De Brito and Silva, 2016).

The economic growth and urban development have also led to an excessive amount of generated waste generated by demolition (Kisku *et al.*, 2017). The construction and demolition wastes (CDW) are typically disposed in landfills, causing contamination of soil and groundwater (Tam *et al.*, 2018). In Canada, the annual CDW production has been estimated at 9 million tons (Yeheyis *et al.*, 2013). Moreover, other parts of the world have reported concerning amounts of generated CDW. For instance, the European Union produces around 0.85 billion tons per year, whereas the USA and China reported 170 and 120 million tons per year, respectively (De Brito and Silva, 2016). The massive amount of generated CDW has posed a serious threat to landfilling space availability. In Canada, the CDW accounts for about 27% of the total waste disposed in landfills (Yeheyis *et al.*, 2013). Also, Duan *et al.* (2013) predicted that in Hong Kong landfills will be depleted by 2021.

Furthermore, the increased urgency of mitigating global warming requires decreasing the carbon dioxide (CO_2) footprint of concrete production (Jiménez *et al.*, 2018). This is a major challenge for the cement industry since it accounts for about 5% of the global CO_2 emissions. The use of supplementary cementitious materials and lower energy alternatives for clinker calcination are a latent solution to overcome the huge amount of CO_2 released to the environment (De Brito and Silva, 2016). Also, Jiménez *et al.* (2018) assessed the resulting CO_2 emitted by different concrete mixtures comparing the emissions produced

by 1 m^3 of concrete containing recycled aggregates and concrete with normal aggregates. They concluded that the replacement of natural aggregates by recycled aggregates can decrease the amount of CO_2 released to the environment by concrete production.

Recycled aggregate concrete (RAC) could contribute to mitigating the depletion of natural aggregates, reducing the carbon footprint of concrete construction, and averting the landfilling of colossal amounts of construction and demolition waste. After World War II, the use of recycled materials in concrete mixtures was initiated. However, it was not until the 1980s that the use of CDW as recycled aggregates gained considerable progress (Tam *et al.*, 2018). As defined by the International Institute for Sustainable Development (2019), sustainable development is development that does not prevent the future generations to meet their needs. Thus, the use of recycled aggregates helps to promote a more sustainable development because the use of less natural aggregates aids better management of these resources and reduces reliance on landfill sites for CDW disposal.

Despite its undisputed environmental advantages, most of the studies on the performance of RAC claim that its use as partial or full replacement for natural aggregates implicates a decrease in the mechanical and durability performance of concrete. Yet, the existing research on the performance of RAC is not yet sufficient to accurately determine to what extent the inclusion of RA contributes to a decline of the concrete properties. Furthermore, the emerging stringent mechanical, durability, sustainability and resilience requirements have brought about the production of more advanced cementitious materials. The use of RA along with a broad variety of supplementary cementitious materials has been considered to meet such needs, resulting in high non-linear relationships between the mixture components and the concrete properties (Arredondo-Rea *et al.*, 2012; Çakır and Sofyanlı, 2015; Corinaldesi and Moriconi, 2009; Pereira *et al.*, 2012).

Typically, statistical methods have been used to model the properties of conventional concrete, such as compressive strength, modulus of elasticity, tensile and flexural strength, etc. (Abdon Dantas *et al.*, 2013). However, with the advent of complex mixtures to meet the demanding requirements of the recent urbanization development, such statistical procedures have demonstrated poor accuracy to determine the engineering properties of

the complex emerging cementitious composites (Deshpande *et al.*, 2016). The inclusion of more ingredients in RAC mixtures has led to highly non-linear relationships between the mixture ingredients and the engineering properties of RAC. Thus, traditional statistical procedures have not been able to capture to what extent these ingredients affect the properties of RAC. Accordingly, the use of more robust modeling, such as machine learning (ML) techniques, is needed to capture the effects of the mixture composition on the properties of concrete. ML techniques have gained substantial attention over the past decades owing to its remarkable capability of data analysis and processing. These algorithms are capable of learning the underlying principles of complex systems and forecasting accurately the related output (Marsland, 2015).

ML is a branch of artificial intelligence that comprises a large number of algorithms. The main objective of these algorithms is to detect patterns within data to then forecast sensitive outputs (Salehi and Burgueño, 2018). These algorithms are categorized in supervised learning, unsupervised learning, and reinforcement learning. The difference among these categories of ML is mainly the distinctness between the available outputs. Whilst supervised learning forecasts data learning from known outputs, unsupervised learning does it with unknown outputs. Reinforcement learning, like unsupervised learning, clusters the data, however, it uses known outputs, as in supervised learning (Marsland, 2015).

Data is passed to ML algorithms in the form of vectors, called input vectors. The input vectors are a D-dimensional collection of features (Murphy, 2012). Depending on the objective of the models, for instance, a model that is aiming at predicting the compressive strength of concrete, these features may correspond to the ingredient's dosage of the mixture. In general, ML algorithms work by taking an input vector to predict an output for such a vector, and then moving to the next input (Marsland, 2015).

ML techniques have gained significant attention in the last decades owing to the versatility of these algorithms and to the recent availability of larger data (Haeb-Umbach *et al.*, 2019). Thus, ML techniques have been applied in different fields of science and industrial development. The recent development of some ML models has attained several achievements, including exceeding human performance in image recognition, or a

developed model from Microsoft that resembled the human aptitudes in speech transcription. In general, ML techniques have proven successful in many applications.

In the civil engineering field, there have been many applications of ML techniques, such as structural health-monitoring, prediction of different properties of concrete, design optimization of structural elements, etc. Data driven ML techniques have proven to be successful in the prediction of RAC mechanical properties including the modulus of elasticity and compressive strength (Behnood *et al.*, 2015; Deng *et al.*, 2018; Deshpande *et al.*, 2016; Khademi *et al.*, 2016). However, the small amount of data employed by existing research compromises the ability of these models to generalize accurately the underlying phenomena involved to predicting the behavior of new sets of input data. Thus, creating reliable and more comprehensive datasets is intended in this dissertation. Furthermore, a novel ML method applied for the first time to predict the carbonation depth of RAC will be deployed.

1.1 Research Objectives

Despite the large amount of research carried out to determine the engineering properties of RAC, the need for more robust models and more diverse datasets is key to developing reliable knowledge on the effects of the inclusion of RA. ML aims at creating models which after learning from certain training datasets can forecast accurate predictions on unseen data never presented to the model, *i.e.*, a model that can generalize (Chollet, 2018). Accordingly, the objectives of the present thesis are outlined below:

1. Conduct an analysis of previous studies on the application of ML methods to predict the compressive strength of novel concrete technologies available in the open literature. Accordingly, determine the advantages and disadvantages of the different algorithms and summarize their achieved performance, highlighting their contributions to the development of mainstream concrete mixtures.
2. Develop a large and reliable dataset for predicting the compressive strength of RAC, ensuring that the ML models created herein can generalize the underlying principles of the compressive strength of RAC.

3. Perform mixture proportioning optimization using ML techniques for different classes of compressive strength of RAC.
4. Develop a ML model to predict the carbonation depth of RAC in view of the growing recognition that the durability-related properties of concrete are affected by the inclusion of RA and compare the carbonation-depth ML model to previous theoretical models that determined it analytically.

1.2 Original Contributions

In this research, a study on the mechanical and durability properties of RAC was conducted. To overcome the difficultness of the highly non-linear relationships between the properties of RAC and its mixture components, ML techniques were applied. The original contributions of the present thesis include:

1. An original literature review of the ML applications to predict the compressive strength of RAC considering that previous literature reviews have analyzed broader applications of ML techniques in civil engineering.
2. Creating one of the largest databases yet to predict the compressive strength of RAC, thus ensuring the generalization capacity of the models developed herein. Other studies have used smaller datasets which can compromise the generalization capability of the resulting models.
3. Applying, for the first time, ML methods to predicting the carbonation resistance of RAC. To the best of the author's knowledge, there is no such application of ML techniques.

1.3 Thesis Structure

The present thesis has been organized following the integrated-article guidelines of the School of Graduate and Postdoctoral Studies (SGPS) at Western University. It includes five chapters that develop a broad analysis and implementation of ML models to determine the performance of RAC by predicting two of its most significant engineering properties: compressive strength and carbonation resistance.

Chapter 1 is an introductory chapter that provides the background of the present study along with the main objectives to achieve.

Chapter 2 provides a critical analysis of the available literature on ML techniques that have been applied to predicting the compressive strength of different mainstream concretes: high-performance concrete, self-compacting concrete, recycled aggregate concrete, etc.

Chapter 3 presents an application of several state-of-the-art ML techniques to predict the compressive strength of RAC. Also, this chapter performs a mixture proportioning of RAC using a particle swarm optimization coupled with a gradient boosting regression tree.

Chapter 4 introduces a gradient boosting regression tree to predict the carbonation depth of RAC and compares the developed ML method to three different theoretical models that aimed at determining the carbonation depth of concrete.

Chapter 5 summarizes the general outcomes and conclusions of the present research.

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Chapter 2

2 Machine Learning Prediction of Compressive Strength of Modern Concrete

Compressive strength is an essential property of concrete since it is a requirement for design and a determinant factor in the load-bearing capacity of concrete structures. Moreover, several mechanical and durability properties of concrete are related with the compressive strength, including the elastic modulus, tensile and flexural strength, shrinkage strains, durability in aggressive environments and resistance to the ingress of hostile substances (Gupta, 2006). The compressive strength of conventional concrete (CC) has been modeled using traditional statistical procedures such as linear and non-linear regression analyses (Abdon Dantas *et al.*, 2013; Chou and Pham, 2013; Hong-Guang and Ji-Zong, 2000). However, emerging stringent mechanical, durability, sustainability and resilience requirements have brought about the production of more advanced cementitious materials. A broad variety of supplementary cementitious materials, fibers and chemical admixtures have been incorporated to meet such needs, leading to more complex microstructure. Hence, the compressive strength of modern advance cementitious composites has become related to a multitude of parameters, through complex non-linear relations.

With the advent of new cementitious composites, such as ultra-high-performance concrete, engineered cementitious composites, geopolymers and alkalis-activated systems, statistical procedures have increasingly demonstrated poor accuracy in modeling the engineering properties of such emerging systems. For instance, Snell *et al.* (1989) found that just with the inclusion of superplasticizer into certain mixture proportions noticeably decreased the capability of statistical models to determine the compressive strength, with a coefficient of determination of 0.10, which is an unquestionably poor accuracy (Snell *et al.*, 1989). Furthermore, modern concretes require complex design considerations. Even mainstream concretes, such as high- and ultrahigh, performance concrete (HPC and UHPC), recycled aggregate concrete (RAC), and self-consolidating concrete (SCC) have complicated mixture design due to the large mixture components. This has led to highly non-linear relationships between the mixture proportions and the compressive strength of concrete.

Additionally, several experimental test must be carried out to better understanding the intricate relationship, which requires substantial time and cost investment (Deshpande *et al.*, 2016).

Artificial intelligence (AI) techniques have recently gained considerable attention owing to its remarkable potential resolving various complex problems. AI refers to computational systems that can act or think rationally (Russell and Norvig, 1995). Machine learning (ML), which is a prominent branch of AI, denotes the capability of computers to learn the underlying mechanism of a complex system and make accurate related predictions (Marsland, 2015). ML encompasses a wide variety of algorithms that can recognize patterns in data (Murphy, 2012). It is generally categorized in three major classes (**Figure 2-1**), including supervised learning, unsupervised learning and reinforcement learning (Mahdavinejad *et al.*, 2018). Supervised learning refers to those algorithms that aim at predicting either a continuous or discrete output, known as regression and classification algorithms, respectively (Murphy, 2012). In supervised methods, the model is trained using data examples with known outputs. In contrast, the target of the unsupervised learning is to identify the relationship within the data without predefined labels for the purpose of clustering (Murphy, 2012). Unsupervised learning models are also known as non-parametric models (Murphy, 2012). The less common type of ML, reinforcement learning, is a type of trial and error learning that bridges the gap between supervised and unsupervised learning as it determines the similarities in the data given correct answers (Marsland, 2015). ML methods have acquired increasing popularity in several scientific fields owing to their ability to learn trends even when there is no noticeable tendency within the data (Chou et al., 2014).

In civil engineering, ML techniques have generated great interest in numerous applications considering their versatility and robust performance. They have been employed for two main purposes, namely optimization and prediction (M.-Y. Cheng *et al.*, 2014; Zewdu Taffese and Sistonen, 2017). A popular application of ML methods is in structural optimization that aims at minimizing the cost of a structure considering given required performance. For instance, the size, topology and shape of structural can be optimized using ML techniques such that the structure meets the design requirements (Aldwaik and

Adeli, 2014). On the other hand, predictive algorithms are developed to learn tendencies from a given dataset and generalize it to provide accurate predictions. In civil engineering, ML methods have been applied to different problems in various fields including geotechnics, fracture mechanics, structural health monitoring, etc. (Adeli, 200; Aldwaik and Adeli, 2014; Amezquita-Sanchez *et al.*, 2016; Arciszewski and De Jong, 2001; Kicinger *et al.*, 2005; Liao *et al.*, 2011; Lu *et al.*, 2012; Mardani *et al.*, 2015; Nasiri *et al.*, 2017; Penadés-Plà *et al.*, 2016; Salehi and Burgueño, 2018; Shahin, 2014). However, prediction of different properties of normal and modern concretes, such as mechanical, thermal, and durability properties, has been addressed in the literature and the predictive accuracy of various algorithms has been explored and reported. In addition to normal concrete, HPC, RAC, SCC, self-healing concrete, etc. have been modeled using ML methods (Abdon Dantas *et al.*, 2013; Chou and Pham, 2013; Gupta, 2006; Hong-Guang and Ji-Zong, 2000; Siddique *et al.*, 2011).

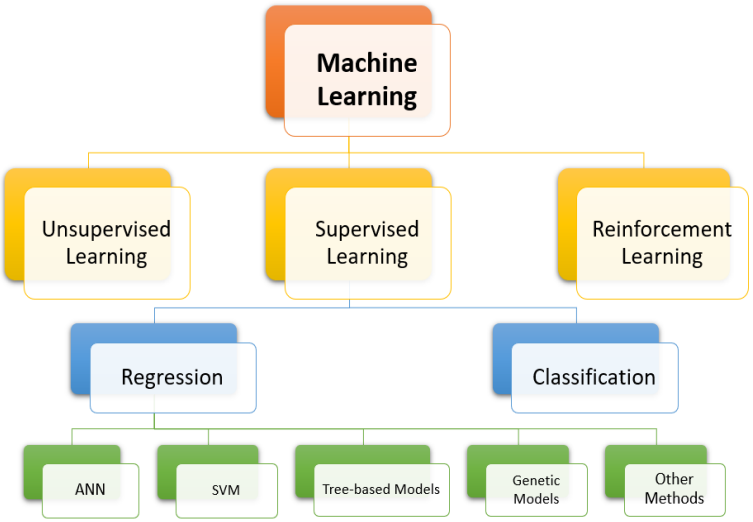

Figure 2-1: Machine learning categories.

The present chapter systematically reviews the applications of ML algorithms in predicting the mechanical properties of modern types of concrete, including HPC, RAC, and SCC. Moreover, a methodical analysis and comparison of different algorithms along with their hyperparameters are conducted. Finally, the limitations of models are distinguished and

recommendations regarding future work are presented. This chapter presents a comprehensive overview of the ML knowledge required to model the compressive strength of the cementitious materials in terms of hyperparameter tuning and evaluation metrics.

2.1 Research Methodology

Initial analysis of 141 pertinent peer-reviewed publications retrieved from the open literature was conducted. The scope of the reviewed was subsequently narrowed to focused on the compressive strength of novel concretes, discarding conventional concrete mixtures. The rationale for this is that the relation between compressive strength and mixture design of normal concrete is rather simple, while that for emerging types of concrete is complex and highly non-linear. Therefore, some articles were discarded from the initial collection as they were beyond the scope of this review. For instance, publications on the application of ML techniques to estimate the compressive strength of conventional concrete were dropped. Furthermore, those studies aimed at predicting concrete properties other than compressive strength were not selected. For instance, papers which employed AI-based methods to predict the shear strength of concrete strengthen with fiber-reinforced polymer were not covered in this thesis. Ultimately, 63 peer-reviewed journal papers were scrutinized herein. The final collection includes papers published in journals of reliable publishers including Elsevier, Springer, ACI, ASCE, etc. **Table 2-1** presents the aforementioned 63 papers.

2.2 Machine Learning for Determining Concrete Compressive Strength

Machine Learning (ML) techniques are highly efficient in data analysis and can be implemented generally without need for rigorous programming (Salehi and Burgueño, 2018). ML algorithms have proven successful in predicting the compressive strength of different types of concrete. This is of great importance to gain understanding of the highly non-linear relations between mixture proportions and engineering properties, without need for laborious trial batches and extensive experimental programs.

Table 2-1: Analyzed references

Conc.	Journal	References	Conc.	Journal	References
RAC	Constr. Building Mater.	Deng *et al.*, 2018	FAC[a]	Comput. Mater. Sci.	Topcu and Saridemir, 2008
Cellular concrete	ACI Materials Journal	M. Nehdi *et al.*, 2001	FAC[a]	Int. J. Appl. Sci. Eng.	Chopra *et al.*, 2015
HPC	Autom. Constr.	M.-Y. Cheng *et al.*, 2012	HPC	Cem. Concr. Res.	I C Yeh, 1998
RAC	Constr. Building Mater.	Abdon Dantas *et al.*, 2013	HPC	Constr. Building Mater.	Chou and Pham, 2013
EFC	J. Build. Eng.	Naderpour *et al.*, 2018	AAC[c]	Comput. Mater. Sci.	Topcu and Saridemir, 2007
RAC	Constr. Building Mater.	Duan *et al.*, 2013	EFC[d]	J. Comput. Civ. Eng.	Omran *et al.*, 2016
RAC	Int. J. Sustain. Built Environ	Deshpande *et al.*, 2014	Cellular Concrete	Constr. Building Mater.	Ashrafian *et al.*, 2020
RAC	Int. J. Sustain. Built Environ	Deshpande *et al.*, 2016	Cellular Concrete	J. Mater. Civ. Eng.	Kiani *et al.*, 2016
CC	Rom. J. Mater.	Baykan *et al.*, 2017	HPC	Constr. Building Mater.	Chou *et al.*, 2014
CC	Cem. Concr. Res.	Hong-Guang and Ji-Zong, 2000	ECC[g]	Constr. Building Mater.	Shi *et al.*, 2018
HPC	J. Comput. Civ. Eng.	Kasperkiewicz *et al.*, 1995	PC[e]	Iraqui J. of Civ. Eng.	Al-Janabi and Al-Hadithi, 2008
HPC	Int. J. Intell. Technol.	Gupta, 2006	UHPC	Mach. Learn. Res.	Choudhary, 2019
HPC	Int. J. Comput. Appl.	Deepa *et al.*, 2010	Rubb. Concrete	WSEAS Trans. Comput.	Van Tittelboom and De Belie, 2013
SCC, HPC	Constr. Building Mater.	Eskandari *et al.*, 2009	SHC[b]	Materials	Suleiman and Nehdi, 2017
HPC	Comput. Struct.	Slonski, 2010	MSC[f]	J. Clean. Prod.	J. Zhang *et al.*, 2020
HSC	Constr. Building Mater.	Oztas *et al.*, 2006	HPC	Eng. Appl. Artif. Intell.	M.-Y. Cheng *et al.*, 2014
HPC	Adv. Eng. Softw.	Mousavi *et al.*, 2012	HPC	Constr. Building Mater.	Behnood *et al.*, 2017
HPC	Autom. Constr.	Khan, 2012	HPC	Constr. Building Mater.	Bui *et al.*, 2018
HPC	Eng. Appl. Artif. Intell.	Erdal *et al.*, 2013	HPC	Eng. Appl. Artif. Intell.	Erdal, 2013
HPC	J. Comput. Civ. Eng.	I C Yeh, 1999	HPC	Constr. Building Mater.	Yu *et al.*, 2018
HPC	J. Comput. Civ. Eng.	Chen and Wang, 2010	HPC	Constr. Building Mater.	Q. Han *et al.* 2019
HPC	Expert Syst. Appl.	Castelli *et al.*, 2013	RAC	Comput. Mater. Sci.	Ilker Bekir Topçu and Saridemir, 2008
HPC	J. Comput. Civ. Eng.	M.Y. Cheng *et al.*, 2014	RAC	Neural Comput. Appl.	Gholampour *et al.* 2018
HSC	J. Mater. Civ. Eng.	Tayfur *et al.*, 2014	HPC	Adv. Eng. Softw.	Mohd. Zain *et al.*, 2005
HPC	Constr. Building Mater.	Chithra *et al.*, 2016	SCC	ACI Materials Journal	Moncef Nehdi *et al.*, 2001

Table 2-1: Analyzed references, continued

Conc.	Journal	References	Conc.	Journal	References
HPC	J. Eng. Res. Appl.	Rguig and El Aroussi, 2017	HPC	Cem. Concr. Res.	Lim *et al.*, 2004
FRP	Compos. Struct.	H. Naderpour *et al.*, 2010	FRP	Compos. Struct.	H Naderpour *et al.*, 2019
FRP	Compos. Part B	Elsanadedy *et al.*, 2012	FRP	Compos. Part B	Jalal and Ramezanianpour, 2012
FRP	Eng. Struct.	Cascardi *et al.*, 2017	SCC	Neurocomputing	Vakhshouri and Nejadi, 2018
SCC	Adv. Eng. Softw.	Siddique *et al.*, 2011	SCC	Constr. Building Mater.	Uysal and Tanyildzi, 2011
SCC	Alexandria Eng. J.	Uysal and Tanyildizi, 2012	Slag and FAC	J. Chin. Inst. Civ. Hydraul. Eng.	I C Yeh, 2003
HPC	J. Comput. Civ. Eng.	Chen, 2003			

[a] Fly ash concrete
[b] Self-healing concrete
[c] Autoclaved aerated concrete
[d] Environmentally friendly concrete
[e] Polymer modified concrete
[f] Manufactured sand concrete
[g] Eng. cementitious composites

To ensure the accurate prediction of ML models, it is crucial to select appropriate hyperparameters. Hyperparameters are user-defined parameters that configure ML models. For example, the number of hidden neurons in artificial neural networks (ANN), the regularization parameter for support vector machine (SVM), the number of trees in tree-based ensembles, are referred to as hyperparameters (Bergstra *et al.*, 2013; Tsirikoglou *et al.*, 2017). Such parameters should be tuned so as the best predictive accuracy can be achieved.

However, there is generally no rigorous mathematical procedure for optimizing hyperparameters that leads to accurate predictions (Oztas *et al.*, 2006). For instance, in the case of ANN, there is no defined rule to determine the appropriate number of hidden neurons or hidden layers (Oztas *et al.*, 2006). Accordingly, the selection of optimum hyperparameters highly depends on both the model and the dataset. Moreover, tuning hyperparameters is an important task to avoid overfitting in the training process so that the model could be generalized for new data (Tsirikoglou *et al.*, 2017). Overfitting is an overestimation or memorizing of the pattern within the training data that results in high accuracy of the training set, and considerably lower accuracy for the testing set (Julien-Charles Lévesque, 2018). Therefore, it is essential to explore the model configuration as well as tuning its hyperparameters to better understand the performance of the applied

algorithm for a specific problem. The various ML algorithms utilized to predict the compressive strength of concrete along with their tuned hyperparameters and data description are reviewed below.

2.2.1 Artificial Neural Networks

ANN is the most commonly used ML technique to predict the compressive strength of different conventional and non-conventional types of concrete mixtures. ANNs mimic the network of biological neurons that constitute the brain (Vapnik, 1998). From a computational point of view, ANN is an adaptive model that learns the influence of the input data to predict the output by a learning process that estimates the weight of every unit called neuron. As shown in **Figure 2-2**, a weight is assigned for each input parameter. Subsequently, a simple computation is performed using the weights and biases together via including bias to generate an input. Finally, the output is calculated using a pre-defined activation function. There are several types of ANN models with different hyperparameters. The importance of each hyperparameter depends on the implemented algorithm and its architecture. In general, the most determining hyperparameters in ANN models are the initial weights, learning rate, number of epochs, activation functions, number of layers, and number of neurons (Chopra *et al.*, 2015). Additionally, momentum becomes important for models using the back-propagation algorithm (BPA), which is the most popular algorithm in ANN models (Erdal, 2013). The hyperparameters of ANN models that have been used to predict the compressive strength of non-conventional concretes are presented in **Table 2-2** (Bui *et al.*, 2018; Cascardi *et al.*, 2017; Chen and Wang, 2010; M.-Y. Cheng *et al.*, 2012; M.Y. Cheng *et al.*, 2014; Chithra *et al.*, 2016; Chopra *et al.*, 2015; Chou and Pham, 2013; Deshpande *et al.*, 2014, 2016; Duan *et al.*, 2013; Elsanadedy *et al.*, 2012; Erdal *et al.*, 2013; Eskandari *et al.*, 2009; Jalal and Ramezanianpour, 2012; Kasperkiewicz *et al.*, 1995; Khan, 2012; Hosein Naderpour *et al.*, 2018; Moncef Nehdi *et al.*, 2001; Omran *et al.*, 2016; Oztas *et al.*, 2006; Siddique *et al.*, 2011; Topcu and Saridemir, 2007, 2008; Uysal and Tanyildzi, 2011; I C Yeh, 1998, 1999, 2003). It can be observed that most researchers used the sigmoid function as activation function. The number of hidden layers was 1 or 2 in most studies, whilst the maximum

number of hidden layers was 10. Additionally, the learning rate ranged from 0.01 to 1; however, 1 was the most used value.

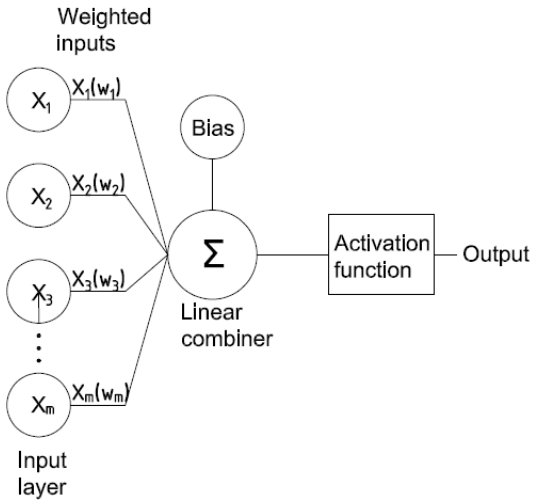

Figure 2-2: Model of a neuron according to Haykin.

2.2.2 Support Vector Machine

SVM models use a data clustering process in which an optimal hyperplane is defined to divide the data. The optimal hyperplane is a subspace that separates the data with greatest gap (**Figure 2-3**). SVM can be used both for regression and classification problems. The main advantage of SVM is that it always finds the global minimum, and thus it is never trapped into local minima, which is a common issue for other models (Lin et al., 2006; Tsochantaridis *et al.*, 2004). However, similar to ANN, the performance of SVM models relies on the optimization of certain hyperparameters, such as the regularization parameter and the kernel function (Gupta, 2006). The most commonly used kernel functions are the linear, polynomial, sigmoid, and the radial basis function (RBF) (Rguig and El Aroussi, 2017). For instance, Yu *et al.* (2018) determined the optimal hyperparameters for SVM model through enhanced cat swarm optimization evolutionary algorithm to predict the compressive strength of HPC. The optimal hyperparameters were the penalty function, $C = 8.9291$, kernel function parameter, $\sigma^2 = 0.3390$, and the intensive loss factor, $\epsilon = 8.9291$. The hyperparameters in studies that used SVM to predict compressive strength of concrete are summarized in **Table 2-3** (M.Y. Cheng *et al.*, 2014; Chou and Pham, 2013; Gupta, 2006; Rguig and El Aroussi, 2017).

Table 2-2: Hyperparameters used in ANN models

Concrete type	Data size	Input	HL[a]	HN[b]	LR[c]	Epochs	LC[d]	MF[e]	AF[f]	References
HPC	1030	8	1	8	1	-	-	0.5	-	Rguig and El Aroussi, 2017
FAC[a]	180	9	1	11	0.75	1000	10000	0.9	Sigmoid	Topcu and Saridemir, 2008
RAC	1178	17	1	3	-	-	1000	-	Hyperbolic tan, linear	Abdon Dantas *et al.*, 2013
RAC	139	6	1	18	-	-	-	-	Sigmoid	Naderpour *et al.*, 2018
RAC	168	14	1	16	0.3	-	10000	0.9	Sigmoid	Duan *et al.*, 2013
RAC	257	9 or 10	1	28-53	-	-	-	-	Sigmoid, linear	Deshpande *et al.*, 2014
RAC	257	9, 5	1	29	-	-	-	-	Sigmoid, linear	Deshpande *et al.*, 2016
CC	49	3	1	50	0.1	3-21325	-	-	Tan-sig, log-sig, linear	Chopra *et al.*, 2015
FAC[g]	27	3	1	50	0.1	2-3713				
HPC	340	6	-	-	-	-	-	-	-	Kasperkiewicz *et al.*, 1995
HPC	187	7	2	5, 3	-	10000	10000	-	Sigmoid	Oztas *et al.*, 2006
HPC	727	8	1	8	1	-	3000	0.5	-	I C Yeh, 1998
HPC and SCC	300	6	2	10 or 5	0.1	2000	-	-	Tan hyperbolic	Eskandari *et al.*, 2009
HPC	-	8	1	6	-	-	-	-	-	Khan, 2012
HPC	80-1133	6-9	3	20, 15, 10	0.01 -0.3	-	-	0.9	Sigmoid transfer	Chou and Pham, 2013
HPC	1030	8	10	10	0.4	1000	-	0.2	-	Erdal *et al.*, 2013
HPC	696	8	1	8	1	-	3000	0.5	-	I C Yeh, 1999
FAC[g], SC[h]	944	8	1	10	1	-	5000	0.5	-	I C Yeh, 2003
HPC	1140	9	1	5	-	-	1000	-	-	Chen and Wang, 2010
HPC	1030	-	1	8	1	-	3000	0.5	-	Cheng *et al.*, 2014
HPC	45	4-6	1	10	-	25-42	-	-	Sigmoid	Chithra *et al.*, 2016
HPC	1133	8	1	20	-	-	-	-	Sigmoid	Bui *et al.*, 2018
RAC	210	8	2	9	0.85	100	30000	0.9	Sigmoid	Ilker Bekir Topçu and Saridemir, 2008
AAC[i]	45	7	2	7,8	0.96	-	-	0.99	Sigmoid	Topcu and Saridemir, 2007
EFC[j]	144	-	1	8	0.1	-	-	0.25	-	Omran *et al.*, 2016
SCC	209	10	2	10,5	0.5	-	-	-	Sigmoid	Moncef Nehdi *et al.*, 2001
SCC	31-168	10	1	14,8	0.04 -0.6	464,61	-	0.1-0.3	-	Uysal and Tanyildzi, 2011
PC[k]	36	4	2	9	0.2	-	-	0.8	Sigmoid	Al-Janabi and Al-Hadithi, 2008

[a] Hidden layers
[b] Hidden neurons
[c] Learning rate
[d] Learning cycles
[e] Momentum factor
[f] Activation function
[g] Fly ash concrete
[h] Slag concrete
[i] Autoclaved aerated concrete
[j] Environmentally friendly concrete
[k] Polymer modified concrete

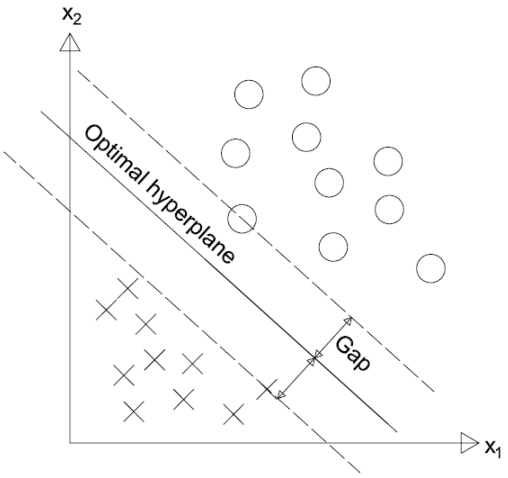

Figure 2-3: Optimal hyperplane separating data with the greatest gap.

Table 2-3: Hyperparameters used in SVM models

Concrete type	Data size	Input	C^a	ε^b	Kernel function type	Kernel parameter	Ref.
HPC	1133	8	10	0.1	RBF	0.1	Chou and Pham, 2013
	104	6					
	80	6					
	194	9					
	144	8					
HPC	1030	8	1	-	-	0.125	M.Y. Cheng *et al.*, 2014
HPC	1030	8	1	-	RBF and Poly	0.125	Rguig and El Aroussi, 2017
HPC	181	6	10	-	RBF	0.5	Gupta, 2006
	190		10	-	Poly	1	

[a] Regularization parameter [b] Regression precision

2.2.3 Fuzzy Logic

Fuzzy logic (FL) is a ML technique originally introduced by Zadeh in 1965 (Zadeh, 1965). It comprises four stages, including fuzzification, fuzzy rule base, fuzzy inference engine and defuzzification (Topcu and Saridemir, 2008). In the first stage, fuzzification, the input data are characterized by a membership function, which returns an intermediary-truth value, a number within the domain of [0,1]. In other words, the membership function demonstrates "how true" the input is, similar to Boolean data in which 1 is considered to be true and 0 to be false (**Figure 2-4**). In the second stage, the fuzzy rules compute the

value assigned by the membership function using rules of the form "if…and…then…else" (Baykan *et al.*, 2017; Topcu and Saridemir, 2008). In the third stage, the inference engine, all the fuzzy rules are taken into consideration, such that all the data are computed into a fuzzy output. Finally, the defuzzification converts the fuzzy output to a real value. The hyperparameters of FL models developed to predict the compressive strength of non-conventional concretes are presented in **Table 2-4** (M.-Y. Cheng *et al.*, 2012; Deshpande *et al.*, 2016; Tayfur *et al.*, 2014; Topcu and Saridemir, 2008; Ilker Bekir Topçu and Saridemir, 2008).

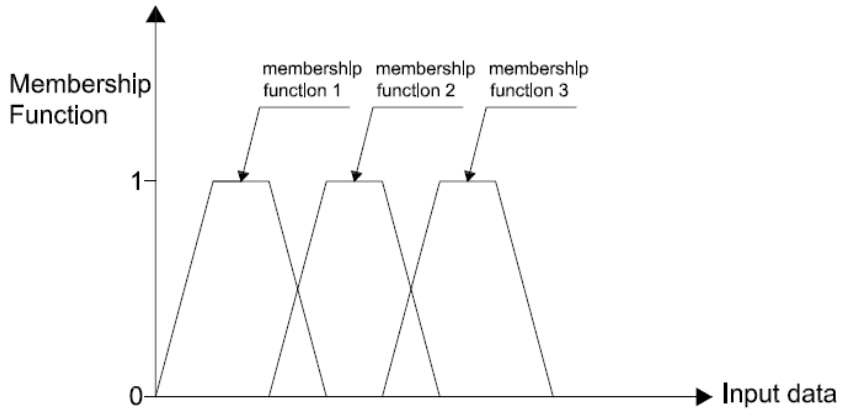

Figure 2-4: Trapezoidal membership function set.

Table 2-4: Hyperparameters used in FL models

Concrete type	Data size	Input	Fuzzy rules	IO[a]	MF[b]	DM[c]	Epochs	References
HPC	1030	8	-	-	Trapezoidal, triangular	-	-	M.-Y. Cheng *et al.*, 2012
Fly Ash Concrete	180	9	Sugeno-type	Product	Triangular	Weighted average	1000	Topcu and Saridemir, 2008
RAC	257	9	Sugeno-type	Product	-	Weighted average	-	Deshpande *et al.*, 2016
	257	5						
HPC	340	6	-	-	-	-	-	Kasperkiewicz *et al.*, 1995
HPC	60	3	Mamdani-type	Min	Triangular	Centroid	-	Tayfur *et al.*, 2014
HPC	1030	8	-	-	-	-	-	Rguig and El Aroussi, 2017
RAC	210	8	Sugeno-type	Product	Triangular	Max-min	100	Iker Bekir Topçu and Saridemir, 2008

[a] Inference operators [b] Membership functions [c] Defuzzification method

2.2.4 Genetic Algorithms

Genetic methods have been successfully applied to predict the compressive strength of different types of concrete. They are inspired by the Darwinian evolution concept of 'survival of the fittest'. Genetic methods represent an alternative to the 'black box' process of many ML techniques, such as ANN (Chen, 2003). Several forms of genetic algorithms have proven to be powerful tools to predict the compressive strength of different types of concrete. The most commonly used genetic methods are gene expression programming (GEP), genetic programming (GP), and genetic algorithm (GA). These methods search for the fittest solution in a population of candidate solutions (Mitchell, 1999). **Figure 2-5** displays the basic flowchart of genetic methods. The main difference between these three methods is the nature of the individuals. In GP and GA, individuals rely solely on their virtues to survive. In contrast, GEP considers phenotypes that allow individuals to survive via external virtues called expression trees. Individuals in GA and GEP methods are linear strings of fixed length, in contrast to GP individuals, which are nonlinear strings of varied size (Ferreira, 2001).

Nonetheless, in most cases, genetic models have not been able to achieve higher predictive accuracy than ANN or evolutionary support vector machine inference (ESMI) models, unless they were combined with other algorithms. For example, Cheng and Wang (2012) combined grammatical evolution with genetic algorithm (GEGA) and compared it with multiple linear regression analysis (MLRA), GA, and back-propagation network (BPN). BPN achieved results 3.6% more accurate for training data set, while GEGA had 4% better results than BPN in the testing set. The general hyperparameters of genetic methods are population of chromosomes (*i.e.* population size), crossover and mutation (Mitchell, 1999). The crossover operator randomly selects two chromosomes to produce two offspring elements according to certain probability, named the crossover rate. Afterwards, the mutation operator flips some of the bits of the chromosome following a given probability, called the mutation rate (Mitchell, 1999). Finally, after both the crossover and mutation have been operated, the population changes to a new offspring, repeating similar steps. The range of hyperparameters in studies that applied GA to predict the compressive strength of

advanced concrete materials are summarized in **Table 2-5** (Castelli *et al.*, 2013; Chen and Wang, 2010; M.-Y. Cheng *et al.*, 2014; M.Y. Cheng *et al.*, 2014; Mousavi *et al.*, 2012).

2.2.5 Hybrid and ensemble procedures

Hybrid procedures can overcome the drawback of relying on proper tuning of hyperparameters associated with most ML techniques. This is of paramount importance since some methods have a strong dependence on the selected hyperparameters, as in the case of FL. Some studies have simply used a supplementary technique to determine the essential tuned value of the hyperparameters for the main model (M.-Y. Cheng et al., 2012). For instance, Vakhshouri and Nejadi (2018) used an adaptive neuro-fuzzy inference system (ANFIS) model to predict the compressive strength of SCC and to emphasize the importance of considering the slump of the fresh concrete as an input factor to obtain better results. ANFIS is a hybrid model that combines ANN and FL. It first characterizes the input data with the use of the membership function, and then converts it to an output using conditional layers.

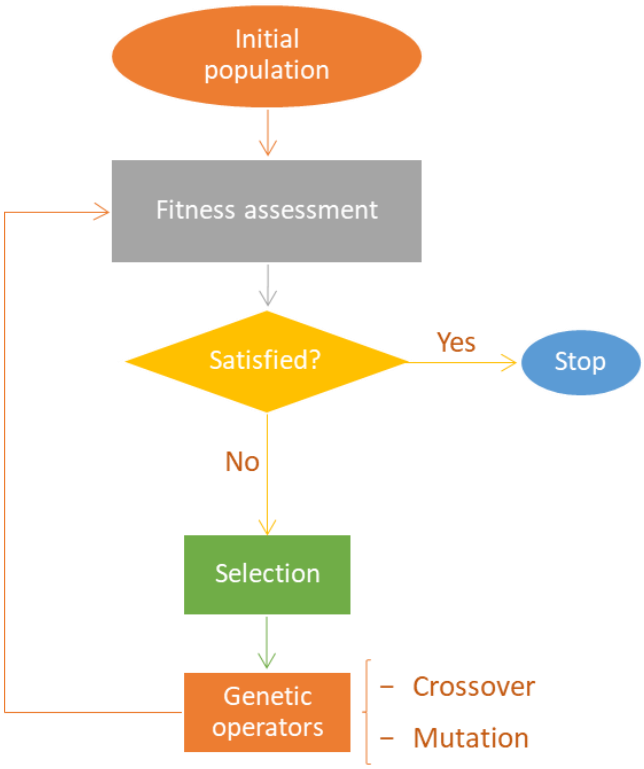

Figure 2-5: Basic flowchart for genetic methods.

Table 2-5: Hyperparameters used in genetic models

Concrete type	Data size	Input	PS[a]	NG[b]	CO[c]	Mutation rate	References
HPC	1133	8	200	2000	0.1	0.044	Mousavi *et al*., 2012
HPC	1140	9	200	1000	-	-	Chen and Wang, 2010
HPC	1028	8	200	2000	0.7	0.3	Castelli *et al.*, 2013
HPC	1030	8	100	2000	0.8	0.05	M.-Y. Cheng *et al.*, 2014

[a] Population size [b] Number of generations [c] Crossover, gene recombination rate

Other studies have explored the ability of ensemble procedures (EP), which are learning algorithms able to reduce variance and increase the predictive capability of fundamental algorithms such as decision trees (Dietterich, 2000; Erdal *et al.*, 2013). The most commonly applied EP algorithm is the bagging method, originally proposed by Breiman in 1994 (Breiman, 1994). Although ensemble methods have demonstrated high predictive accuracy in different fields, they have been less utilized in concrete technology domain. Hence, dedicated research is needed to explore their potential in modeling engineering properties of concrete.

2.2.6 Deep Learning

Deep learning (DL) is a powerful ML algorithm first proposed by Hinton (Dietterich, 2000; Erdal *et al.*, 2013). The fundamental structure of DL is a multilayered ANN (Deng *et al.*, 2018). These types of algorithms have gained significant attention in recent years owing to their powerful ability to solve highly complex problems (S. Han et al., 2019). However, most applications of DL models in civil engineering problems are limited to crack detection or structural health monitoring because it usually needs larger datasets to yield promising results (Cha *et al.*, 2017; Dung and Anh, 2019; Jang *et al.*, 2019; Kim and Cho, 2019; Toh and Park, 2020; Ye *et al.*, 2019; X. Zhang *et al.*, 2019). Accordingly, one paper in the open literature employed DL method to estimate compressive strength of RAC and compared it to other ML techniques such as SVM and back-propagation neural network (BPNN). The authors performed experimental work to obtain the datasets used to construct the models. Although they used a relatively small dataset, their results demonstrated the superiority of convolutional neural networks since they average error for the 28-day compressive strength was 6.63, 4.35, and 6.65 for BPNN, SVM, and DL, respectively (Nair and Hinton, 2010).

2.3 ML Applications for Predicting Concrete Compressive Strength

2.3.1 ML Prediction of HPC Compressive Strength

High-performance concrete (HPC) has been widely used owing to its superior mechanical and durability properties compared to conventional concrete (CC) (I C Yeh, 2003). However, its mixture design includes various supplementary cementitious materials and chemical admixtures, which also affects its compressive strength in quite a complex and difficult manner (Aïtcin, 2004). Therefore, several researchers have explored using ML techniques to either optimize the mixture design of HPC or predict its compressive strength for a given mixture proportions.

To model HPC mixture design using fuzzy-ARTMAP network and predict its compressive strength Kaperkiewicz *et al.* (1995) encountered insufficient data and limited input features. Thus, their dataset had similar input features to models used for predicting the compressive strength of CC. However, they demonstrated the capacity of data-driven models to predict the compressive strength of HPC with desirable accuracy (Kasperkiewicz et al., 1995). I C Yeh (1998) had significant contributions to the application of ML techniques for advanced concretes, especially HPC. In a first attempt to predict the compressive strength of HPC, Yeh proved ANN models to be sufficiently accurate, despite deficiencies in the available data. One of the major findings of this work was that ANN models can be a powerful tool to analyze the effects of each input feature. For instance, using the developed ANN model, the effect of the water-to-binder ratio and the age of testing on the compressive strength of HPC (I C Yeh, 1998) could be analyzed. In a similar study, I C Yeh (1999) used ANN models to predict both the compressive strength and workability of HPC. A software named “High-performance concrete design package using neural network and nonlinear programming (HPC2N)” was developed to perform the mixture design of HPC (I C Yeh, 1999), which was later extended to fly ash and slag concrete. Added to high accuracy in compressive strength prediction, there was significant improvement in learning since ANN could converge after 200 iterations, demonstrating relatively low computational cost (I C Yeh, 2003).

The database published by Yeh was further studied by others aiming to improve the performance of ANN models. Slonski (2010) optimized ANN architecture in terms of number of hidden neurons. Using statistical and Bayesian approaches, an architecture of eight input neurons, ten hidden neurons and one output was proposed [8-10-1] as most accurate (Slonski, 2010). Nevertheless, this required very high computational cost, in contrast to simpler architectures with a smaller number of hidden neurons (eight input neurons, eight hidden neurons, and one output neuron, [8-8-1]), which yielded similar results (Slonski, 2010). Erdal *et al.* (2013) examined the effect of bagging and gradient boosting ensemble techniques coupled with ANN models to predict the compressive strength of HPC using the same dataset. Accordingly, both models performed better than the conventional ANN since the coefficient of determination of the ANN model was $R^2 = 0.9088$, and the corresponding R^2 for ANN and gradient boosting were equal to 0.9278 and 0.9270, respectively (Erdal et al., 2013).

Other studies in the open literature utilized the same dataset to develop predictive models using other techniques. For instance, Castelli *et al.* (2013) introduced geometric semantic genetic programming (GSGP) model to predict the compressive strength of HPC. They compared GSGP to other ML and statistical methods, such as SVM, radial basis function (RBF) network, linear regression (LR), genetic programming (GP), and ANN. The GSGP model outperformed the other models in terms of accuracy. For instance, it had 11.7% higher accuracy compared to SVM using a fourth-degree kernel (Castelli et al., 2013).

The main purpose of the mixer design of HPC is to achieve performance requirements, including compressive strength and workability at lowest cost. Mohd. Zain *et al.* (2005) developed an expert system called HPCMIX for determining HPC mixture proportions. The software, which comprises three modules where the user can design the mixture, adjust it, then estimate its cost, proved useful for mixture proportioning and optimization purposes (Mohd. Zain *et al.*, 2005). M. Y. Chen *et al.* (2014) optimized the mixture design of HPC using GA-ESIM algorithm. They first compared evolutionary support vector machine inference model (ESIM) to ANN and SVM models. They demonstrated that ESIM was more accurate for predicting HPC mixture proportions, with 7.2% higher accuracy compared to other algorithms. Moreover, they optimized HPC mixture proportions using

K-means chaos genetic algorithm (KCGA) coupled with ESIM and provided a design example using the software [48].

ANN is the most widely used AI approach for predicting the compressive strength of different types of concrete (Chithra *et al.*, 2016; Eskandari *et al.*, 2009; Khan, 2012; Oztas *et al.*, 2006; Tayfur *et al.*, 2014; I C Yeh, 1998, 1999). For instance, Eskandari *et al.* (2009) used ANN models to predict the compressive strength of both HPC and self-compacting concrete (SCC). The best network architectures for SCC and HPC were [10-10-5-1] and [9-9-5-1], respectively (Eskandari et al., 2009). Other studies developed ANNs for HPC incorporating specific cementitious materials such as nano-silica, coper slag, and silica fume (Chithra *et al.*, 2016; Khan, 2012). For instance, Khan (2012) demonstrated, using ANN models, that the ideal silica fume dosage was 10%. The ANN model also indicated that the incorporating silica fume brings advantages to concrete, including lower permeability and chloride ions penetration.

Several studies employed fuzzy logic (FL) techniques to model cementitious composites (M.-Y. Cheng *et al.*, 2012; Deshpande *et al.*, 2016; Kasperkiewicz *et al.*, 1995; Rguig and El Aroussi, 2017; Tayfur *et al.*, 2014; Topcu and Saridemir, 2008; Ilker Bekir Topçu and Saridemir, 2008) and predict the compressive strength of HPC (M.-Y. Cheng *et al.*, 2012; Kasperkiewicz *et al.*, 1995; Rguig and El Aroussi, 2017; Tayfur *et al.*, 2014; Topcu and Saridemir, 2008). For instance, Tayfur *el al.* (2014) predicted the compressive strength of HPC using both FL and ANN and found that ANN was 15% more accurate (Tayfur *et al.*, 2014).

M. Y. Cheng *et al.* (2014) compared the genetic weighted pyramid operation tree (GWPOT) to other models including ANN, SVM, ESIM, GOT and weighted operation structure method. GWPOT outperformed all models except ESIM. However, ANN and ESIM are considered “black box” systems, while genetic models can provide explicit equations that show clearly how predictions are made (M.-Y. Cheng *et al.*, 2014).

Tree-based ensembles are popular ML methods to solve regression problems. Such methods have been applied to predict the compressive strength of HPC. Q. Han *et al.* (2019) used a variable optimization method to determine the influencing input parameters in the

prediction of HPC compressive strength. They used different combinations of such parameters to posteriorly run several trial models. The most determinant parameters were the specimen age and water-to-binder ratio. It was concluded that there was significant improvement in prediction of HPC compressive strength after optimization of the input parameters, which achieved lower mean absolute error, $MAE = 3.1055$ MPa, compared to several previous studies that used the same dataset (Chou *et al.*, 2014; Chou and Pham, 2013; Erdal *et al.*, 2013; I C Yeh, 1998).

Deepa *et al.* (2010) used M5P tree-based model to predict the compressive strength of HPC and compared it to both regression and multilayered perceptron (MLP) models. They reported that the accuracy of tree-based model outperformed the other two models based on their root squared mean error ($RMSE$), which was 9.9054, 11.1066, and 7.1874 MPa for MLP, linear regression and M5P models, respectively.

Hybrid procedures along with ensemble models are an alternative to overcome the disadvantages of single-technique models. For instance, Erdal (2013) investigated the prediction performance of single-ensemble and two-level-ensemble techniques using gradient boosting (BG), random subspaces (RS), and bagging algorithms. The combination of BG-RS and bagging-RS improved the accuracy of single decision tree model by 10.99%. Hybrid procedures, on the other hand, are combination of two or more different ML techniques. Rguig and El Aroussi (2017) applied weighted support vector machine (WSVM) to predict HPC compressive strength. WSVM combines SVM with FL, such that the weight of each data point is determined by the FL membership function. Thus, FL performs similar to a filter for input data having noise, before executing the SVM (Rguig and El Aroussi, 2017). WSVM was 10.15% more accurate than simple SVM. Likewise, Bui et al. (2018) introduced firefly algorithm (FFA) coupled with ANN. FFA determined the optimized initial weights and biases prior to performing the final ANN model. This improved prediction accuracy because the initial values of the weights and biases influence the accuracy of ANN models.

2.3.2 Prediction of SCC Compressive Strength

Self-consolidating concrete (SCC), a special class of HPC, emerged in the 1980s (Siddique *et al.*, 2011). SCC can flow and consolidate under its own weight without need for mechanical vibration (Uysal and Tanyildizi, 2012; Uysal and Tanyildzi, 2011). Its more complex mixture design involving various mineral fillers and chemical admixtures makes optimizing SCC mixture proportions and predicting its engineering properties intricate. Striking a balance between flow, passing ability, stability, mechanical strength, durability and sustainability requirements needs powerful predictive tools. Thus, application of ML techniques for this purpose are promising.

Moncef Nehdi *et al.* (2001) were the first to use ML in predicting the compressive strength of SCC. They reported that ANN could successfully predict not only the compressive strength, but also other properties of SCC including segregation, slump flow, and filling ability (Moncef Nehdi *et al.*, 2001). Due to limited data at the time, predictions of these properties were performed separately. Other researchers predicted SCC compressive strength using ANN algorithms. For instance, Siddique *et al.* (2011) predicted the compressive strength of SCC at different ages along with the importance factors of the input data. Uysal and Tanyildzi (2011) compared two learning algorithms including Fletcher power conjugate and Levenberg-Marquardt backpropagation algorithm. They concluded that the Fletcher algorithm had higher accuracy as its coefficient of determination, R^2, was 0.95 compared to that of Levenberg-Marquardt which was 0.92. In another study, Uysal and Tanyildzi (2012) predicted the mixture proportions of SCC using multiple-output architecture and single output architecture. Although running one model to predict multiple outputs required less computational time compared to running several models each aiming at predicting one output, the ANN model with single output architecture led to better results.

2.3.3 Prediction of RAC Compressive Strength

Recycled aggregate concrete (RAC) is an eco-friendly type of concrete that uses processed construction and demolition waste (CDW) as recycled aggregate (RA). In pursuit of sustainability, three main problems are resolved via incorporation of RA into concrete:

environmental problems associated with the disposal of demolition waste, shortage of virgin raw materials for producing conventional natural aggregates, and the environmental footprint generated by the extraction of natural aggregates (Duan *et al.*, 2013; Hosein Naderpour *et al.*, 2018; Yeheyis *et al.*, 2013). However, the heterogeneous nature of RA has led to highly non-linear relationships between RA addition and mechanical properties of RAC. One of the major causes of heterogeneity is that the demolished concrete, except for the residuals of laboratory test, is usually contaminated with materials such as glass, metal, bricks, stones, paper, etc. (Duan *et al.*, 2013). Furthermore, the old mortar adhered to the RA results in weak bond between the aggregates and the cement paste, which is critical zone for the strength of RAC (Deshpande *et al.*, 2014).

Topcu and Saridemir (2007) applied ML techniques to predict RAC compressive strength. Initially, they studied the properties of waste autoclaved aerated concrete (WAAC) at different replacement levels using ANN models. The maximum reduction in predicted properties (compressive strength, modulus of elasticity and ultrasound pulse velocity) occurred at 100% aggregate replacement (Topcu and Saridemir, 2007). In other studies, Topcu and Saridemir, (2008); and Ilker Bekir Topçu and Saridemir (2008) determined that FL and ANN models were powerful tools to predict RAC and fly ash concrete compressive strength with high accuracy despite the limited available data (Topcu and Saridemir, 2008; Ilker Bekir Topçu and Saridemir, 2008). In both studies, they found that ANN had slightly better prediction accuracy than FL. The coefficients of determination for RAC and fly ash concrete were 0.9972 and 0.9984, respectively for ANN models, and 0.9986 and 0.9959, respectively for FL models.

There have been numerous studies that successfully predicted the compressive strength of RAC using ANN methods (Abdon Dantas *et al.*, 2013; Deshpande *et al.*, 2014, 2016; Duan *et al.*, 2013; Hosein Naderpour *et al.*, 2018). Duan *et al.* (2013) proposed [14-16-1] architecture for ANN algorithm to predict RAC compressive strength. They used other characteristics of RA, such as the saturated surface dry mass, water absorption, and volume fraction of coarse aggregate as input parameters. They evidenced that these parameters are useful to predict the compressive strength of RAC (Duan et al., 2013). Additionally, Deshpandae *et al.* (2014) developed various models, including ANN, model tree and non-

linear regression, to predict the compressive strength of RAC. They studied the change in predictive accuracy by adding different non-dimensional input parameters, such as the water-to-total-material ratio, and aggregate-to-cement ratio. Their results revealed that ANN model had superior performance such that the coefficient of correlation was 0.93, 0.85 and 0.82 for ANN model, model tree and non-linear regression, respectively. Similarly, Deshpande *et al.* (2016) reported that ANN models could better predict the compressive strength of RAC in comparison to ANFIS and multiple linear regression models, though the ANFIS model indicated promising performance (Deshpande *et al.* 2016).

Other ML algorithms have been employed to model the mechanical properties of RAC. Omran *et al.* (2016) compared the predictive performance of seven individual ML techniques, including M5 algorithm, REPTree, M5-Rules, decision stump, SMOreg, ANN and Gaussian processes regression, as well as bagging and additive regression ensembles. They used a dataset to predict the compressive strength of a so called environmentally friendly concrete (Omran *et al.*, 2016). The Gaussian process regression outperformed the other techniques. The authors reported the computational time required for each technique and concluded that ANN needed longer time to be executed (Omran *et al.*, 2016). In a different study, Gholampour *et al.* (2018) utilized three regression techniques, including least squares support vector regression (LSSVR), multivariate adaptive regression splines (MARS), and M5 model tree, to predict the compressive strength, flexural strength, elastic modulus, and splitting tensile strength of RAC. They indicated that LSSVR had higher predictive accuracy compared to other models, achieving 13.07% and 14.28% better accuracy compared to that of MARS and M5 model tree, respectively. Also, J. Zhang *et al.* (2020) used a hybrid procedure to determine the compressive strength of manufactures-sand concrete. They used a firefly model to optimize the hyperparameters of three different algorithms: single regression tree, gradient boosted regression three different tree algorithms: single regression tree, gradient boosted regression tree and random forest. Their results indicated that gradient boosted regression tree achieved 1% higher coefficient of correlation, proving to be slightly better than the other models (J. Zhang *et al.*, 2020).

2.3.4 ML Prediction of Compressive Strength of other Concrete Types

Machine learning techniques have been applied to other types of concrete, such as fiber-reinforced concrete, FRP-confined concrete, polymer-modified concrete, cellular concrete, engineered cementitious composites, and rubberized concrete. However, limited pertinent studies could be found in the open literature. Generally, the mechanical strength of these types of advanced concretes is more complex, involving a multitude of non-linear relations, and hence, their mechanical properties are more difficult to predict. Nonetheless, ML techniques have demonstrated to be successful in the prediction of the compressive strength of these types of concretes.

2.3.4.1 Concrete Confined in Fiber-Reinforced Polymer

Fiber-reinforced polymer (FRP) confinement of concrete is widely used as a reinforcing and retrofitting system for damaged structures (H Naderpour *et al.,* 2019). FRP can be used as exterior jacket that performs as passive reinforcement (H Naderpour *et al.,* 2019). Typical regression analyses could not achieve high accuracy in predicting the compressive strength of FRP confined concrete specimens (H. Naderpour *et al.*, 2010). Thus, several studies have successfully applied ANN models (Cascardi *et al.*, 2017; Elsanadedy *et al.*, 2012; Jalal and Ramezanianpour, 2012; H. Naderpour *et al.,* 2010) for this purpose. For instance, Naderpour *et al.* (2010) determined the compressive strength of FRP confined concrete specimens using ANN models. An iterative approach was used to acquire optimal model parameters and concluded that the best number of hidden neurons was 11. On average, the coefficient of correlation, r, achieved by the model was 0.948 (H. Naderpour *et al.*, 2010). Comparing ANN and linear regression models, Elsanadedy *et al.* (2012) emphasized the lack of accuracy of linear regression models to predict the compressive strength of FRP confined concrete. Accordingly, the coefficient of determination, R^2, for ANN model was 0.94, while it was 0.73 using linear regression, which demonstrates significant improvement in ANN predictive accuracy (Elsanadedy *et al.*, 2012). In another comparison of ANN models to regression analysis, Jalal and Ramezanianpour (2012) found ANN models to be more accurate compared to statistical linear regression, non-linear regression, and second order models in determining the compressive strength of FRP

confined concrete. The authors reported an average error of 10.66% for ANN models and at least 14.44% for regression analysis (Jalal and Ramezanianpour, 2012). Moreover, Cascardi *et al.* (2017) determined an analytical relationship for a confinement coefficient, *k*, that related the compressive strength of FRP confined concrete to that of unconfined concrete using ANN. The ANN model resulted in a correlation coefficient of 0.80 and 0.90 for the training and testing datasets, respectively (Cascardi *et al.*, 2017).

2.3.4.2 Cellular Concrete

Cellular concrete is a low-density cementitious material that consist of cement mortar with performed foam in the form of bubbles to create homogeneous cellular structure (M. Nehdi *et al.*, 2001). In addition to its lighter weight compared to conventional concrete (CC), the inclusion of air bubbles provides cellular concrete with superior acoustic and heat insulation (Ashrafian *et al.*, 2020). However, the mechanical properties of cellular concrete are difficult to quantify. For instance, not only could the reduction of density significantly affect the compressive strength of cellular concrete, but also the mixture proportions have a considerable impact on the compressive strength, including the water-to-bonder ratio, foam volume, sand content, and cement content (Ashrafian *et al.*, 2020; Kiani *et al.*, 2016). To overcome such complexities, Nehdi *et al.* (2001) used ANN models to predict the density and compressive strength of cellular concrete. Although the available data was limited, the developed model demonstrated high prediction capability, with compressive strength prediction error of the ANN model at least 47% less than the compressive strength by empirical methods. Additionally, Kiani *et al.* (2016) identified that the main parameters that affect the compressive strength of cellular concrete are the water-to-binder ratio and the foam volume. They reported R^2 between 84.7% and 89.8% for all models. Ashrafian *et al.* (2020) determined the compressive strength of cellular concrete using multivariate adaptive regression splines applying water cycle algorithm (MARS-WCA), and compared it to multiple linear regression, ANN, standard multivariate adaptive regression splines, and support vector regression models. MARS-WCA performed on average 25% better than all the other algorithms.

2.3.4.3 Engineered Cementitious Composites

Engineered cementitious composites (ECC) are characterized by their high ductility (M.M. and V.C. Li, 1994) and unique ability to resist higher levels of strain without failure. Ductility in these composites is achieved via inclusion of short high-performance fibers or functional particles in the mixing process. Consequently, the specification of ECC mixture components is a convoluted design process (Shi *et al.*, 2018). Shi *et al.* (2018) created an ANN model to predict different properties of ECC including flexural and compressive strength. The maximum error of compressive strength prediction was 4% proving the capacity of ML models to accurately predict the mechanical properties of advanced cementitious composites.

2.3.4.4 Polymer Modified Concrete

Polymer modified concrete is a type of concrete that includes water soluble of emulsified polymer as an admixture (Mahmood Al-Janabi and Abdulwahab Al-Hadithi, 2008). Adding polymers to the concrete mixtures can lead to improvement in durability of concrete and an increase in compressive strengths. Mahmood Al-Janabi and Abdulwahab Al-Hadithi, (2008) determined the compressive strength of polymer modified concrete using different ANN models. They reported a coefficient of correlation, r, of 0.89, 0.87, and 0.81 for the training, testing and validation data sets, respectively.

2.3.4.5 Ultra-High-Performance Concrete

Ultra-high-performance concrete (UHPC) has superior engineering properties and its suitable for more sophisticated structures (Graybeal, 2006). Choudhary (2019) created an ANN model to predict the compressive strength of UHPC and to implement a sequential feature selection analysis. After performing feature selection, the input parameters retained to predict the UHPC compressive strength were cement, silica fume, fly ash, and water content. A coefficient of determination, R^2, of 0.991 was reported for UHPC compressive strength prediction.

2.3.4.6 Rubberized Concrete

Rubberized concrete is environmentally friendly concrete that incorporates granules from recycled scrap tire rubber as aggregate. Advantages of rubberized concrete include decreased unit weight and more ductile behavior (I B Topçu and Uygunoglu, 2016). Abdollahzadeh et al. (2011) explored the compressive strength of rubberized concrete using ANN and multi linear regression. ANN model achieved more accurate prediction of rubberized concrete compressive strength with a coefficient of correlation of 0.9823, compared to 0.74 for multi linear regression (Abdollahzadeh *et al.*, 2011).

2.3.4.7 Self-Healing Concrete

Concrete could heal fine cracks intrinsically owing to chemical reactions such as carbonatation of calcium hydroxide or hydration of clinker materials (Van Tittelboom and De Belie, 2013). Some researchers reported that addition of certain healing agents including supplementary cementitious materials, crystalline additives or biochemical agents can improve autogenous self-healing in concrete (Suleiman and Nehdi, 2017). However, the healing process involves various complex chemical and physical mechanisms and is difficult to predict (V.C. Li and Herbert, 2013). Therefore, Suleiman and Nehdi (2017) explored the feasibility of a hybrid genetic algorithm-artificial neural network (GA-ANN) to predict the self-healing ability of concrete in terms of the parameters involved, with a coefficient of determination, R^2, of 0.99765, 0.99773, and 0.99736 for training, validation, and testing data sets, respectively (Suleiman and Nehdi, 2017).

2.4 Discussion and Recommendations

To effectively use machine learning (ML) techniques in predicting the compressive strength of non-conventional concretes, the input data, the selected model and the hyperparameters are key factors to achieve desirable accuracy. Most studies in the open literature used the mixture proportions of the concrete along with the testing age as key input features. Therefore, the ingredients of conventional concrete (CC) including mixing water, cement, fine aggregate, and coarse aggregate contents have been the common input parameters. For HPC and RAC, 44.1% and 29% of the input parameters in the studies

reviewed herein, respectively, correspond to mixture components of CC (**Figure 2-6**). The remaining input parameters depend on the type of the target concrete. For instance, in the case of HPC, the common input parameters are the additions used to enhance the characteristics of HPC, i.e. supplementary cementitious materials, which represent about 32% of input parameters in all models proposed in the literature. Regarding RAC, the input parameters related to the characteristics of the recycled aggregates (RA) represented about 26.2% of the total input features considered in all models analyzed herein. The input parameters are usually scaled using functions with a domain between 0 and 1, or -1 and 1. For instance, the input data for ANN models should be scaled to the domain of [-1,1] so that it can be recognized by the sigmoid function (Bui *et al.*, 2018; M.Y. Cheng *et al.*, 2014; Deepa *et al.*, 2010; Deshpande *et al.*, 2016; Elsanadedy *et al.*, 2012; Eskandari *et al.*, 2009; Hong-Guang and Ji-Zong, 2000; Kasperkiewicz *et al.*, 1995; Hosein Naderpour *et al.*, 2018; Moncef Nehdi *et al.*, 2001).

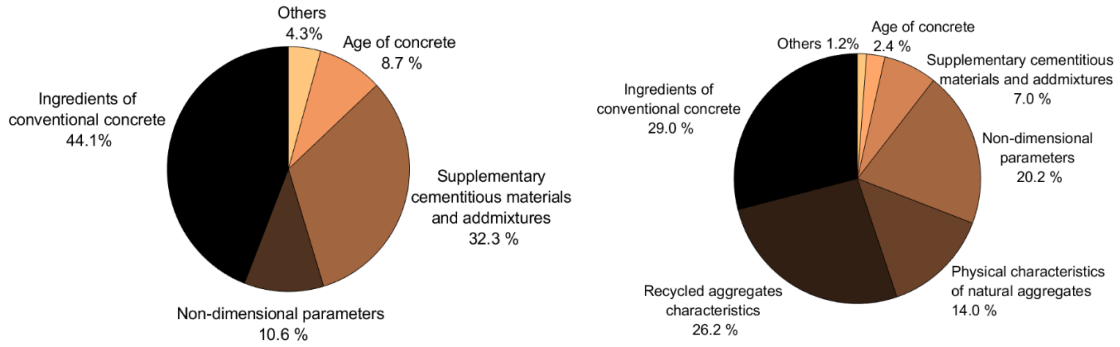

Figure 2-6: Input parameters used for ML models in the prediction of HPC (left) and RAC (right).

One important metric of ML models is feature importance. Some researchers investigated the influence of each input attribute on the predicted compressive strength though sensitivity analyses (Deshpande *et al.*, 2016). Sensitivity analysis determined to what extent each input feature influences the prediction of the output through computing a sensitivity measure (Cortez and Embrechts, 2013). Depending on the type of model, sensitivity analysis can be carried out using different methods. For example, the sensitivity analysis of ANN models can be performed using several techniques, such as the partial derivatives method, the weights method and the classical stepwise method (Park *et al.*,

2007). Hosein Naderpour et al. (2018) computed the importance of each input feature through the importance of weights method and concluded that the water-to-total-material ratio and the water absorption capacity of the aggregates were the most influential input features to predict the compressive strength of RAC. However, in genetic algorithms, an easy approach to sensitivity analysis is to determine the frequency of appearance of the input parameters (in percentage). Accordingly, a value of 1.0 (100%) denotes that the input value appeared in all solutions, and thus, is a parameter of dominant influence in the predictions (Mousavi *et al.*, 2012). This was the approach that Mousavi et al. (2012) used to determine the input importance, concluding that the water content, cement content and testing age were determinant input features for HPC compressive strength prediction.

Correlation coefficients are used to identify dependency within the input parameters. This is of special importance in the case of genetic algorithms since high dependent values cause the algorithm in the early stages not to change significantly from one generation to another, making the algorithm identify a solution that is not optimal. Therefore, determination of the input correlation coefficients is beneficial to deciding whether certain input parameters should be used (Mousavi *et al.*, 2012).

Cross-validation is a statistical technique that prevents overfitting by subset selection (Picard and Cook, 2010). It is based on the principle that the performance of a model is likely to overfit when it is tested on the same data used to create it (Fonseca-Delgado and Gomez-Gil, 2013). Monte Carlo and k-Fold cross-validation are common methods among subset selection approaches (Picard and Cook, 2010). However, k-Fold cross-validation was the most popular technique among the papers dedicated to predicting the compressive strength of advance concretes. This technique consists of dividing the data into *k* segments and perform the model k-times over these segments (Dietterich, 1998). Several authors applied this technique to their models (e.g., Bui *et al.*, 2018; M.Y. Cheng *et al.*, 2014; Chou *et al.*, 2014; Omran *et al.*, 2016; Siddique *et al.*, 2011; Tayfur *et al.*, 2014)

Most ML techniques have proven to be accurate in predicting the compressive strength of non-conventional concretes. **Figure 2-7** describes the rate of use of ML techniques and statistical analysis within the studies concerning this review. However, the selection of an

appropriate technique depends on the available dataset, along with the objectives of the study. For instance, ANN algorithms have excellent of predicting compressive strength. Yet, being a "black box" model is a considerable disadvantage. Other ML techniques, such as decision trees, avoid the unclarity of the "black box" models and their results are easy to interpret (M.-Y. Cheng *et al.*, 2014). Yet, the accuracy of decision tree models was found to be less than that of ML techniques, especially tree-based ensembles. A brief discussion of the advantages and disadvantages of ML techniques is outlined in **Table 2-6.** Based on the analyses performed in the present review and noting that the selection of the ML model depends on the purpose of the study along with the available dataset, it is recommended to first use ANNs to extend an existing model to a different dataset. ANN, especially that using RBF algorithm, can accurately predict outputs from different input datasets (Nasiri *et al.*, 2017). Furthermore, genetic algorithms are recommended if the purpose is to optimize an equation that describes the compressive strength (Chen and Wang, 2010; M.-Y. Cheng *et al.*, 2014; Mousavi *et al.*, 2012).

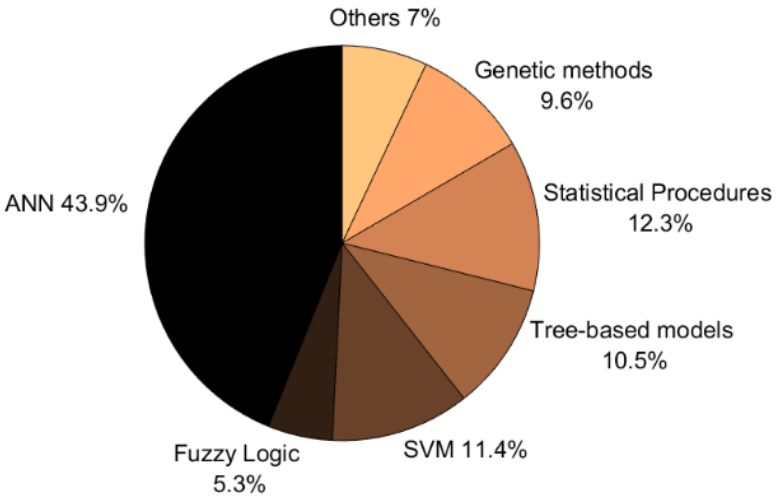

Figure 2-7: Percentage of use of the reviewed ML methods in the open literature.

A comparison of the prediction accuracy of various models proposed in the literature and reviewed herein is presented in **Table 2-7** to **Table 2-13** for those studies that reported coefficient of determination, R^2, as an evaluation metric for the developed ML. While ensemble methods and deep learning techniques have not been extensively applied to model concrete materials, they have generally outperformed other techniques in terms of

both accuracy and speed (Salehi and Burgueño, 2018). Therefore, deep learning and ensemble methods seem to be most promising for future studies in this field and deserve further investigation.

Table 2-6: Advantages and disadvantages of ML techniques

Technique	Advantages	Disadvantages
Artificial Neural Network	• Able to predict accurately even when working with poor or corrupted data • Non-linear mapping properties • Self-adapting model to different environmental conditions • Parallel processing capabilities • Due to its generalization capability, ANN models can predict accurate results of experiments other than the ones it was trained for	• High computational cost • The number of iterations is often in the order of thousands • The convergence rate is dependent on the choice of the values of learning and moment ratios • Lack of generalization when the number of samples is limited • Considered black box systems due to the lack of clarity in their prediction process
Support Vector Machine	• Can overcome the problem of small sample size • Always identifies a global minimum and not a local one • Requires smaller computational time than ANN models	• High dependence on the selected weighting function • Less accurate than ANN models
Genetic Algorithms	• Adapts to changing environments • Ability to handle various types of objective functions (root mean square error, sum squared error, etc.) • Overcomes the disadvantage of the black box algorithms	• Once the individuals have a similar structure, the results do not change much, leading to early convergence • Less accurate than ANN models
Fuzzy Logic	• A powerful tool to simulate non-linear behavior • The IF-THEN rules can model qualitative human-like reasoning without performing quantitative analyses	• Require very large data set • Relies in large number of hyperparameters to obtain accurate results
Decision Trees	• Merging predictor categories help to avoid overfitting	• Significant less accurate results that most methods
Hybrid procedures	• In general Hybrid methodologies are more accurate than most ML techniques	• Choosing an appropriate ML technique, and designing the model architecture is important to obtain precise predictions

Table 2-7: Coefficient of determination of compressive strength prediction using statistical regression models

Concrete	Model	R^2	References
RAC	Non-Linear Regression	0.6909	Deshpande *et al.*, 2014
RAC	Multi Linear Regression	0.6085	Deshpande *et al.*, 2016
HPC	Non-Linear Regression	0.8199	Mousavi *et al.*, 2012
	Linear Regression	0.6477	
HPC	Linear Regression	0.6592	Chithra *et al.*, 2016
Cellular Concrete	Multiple Linear Regression	0.7525	Ashrafian *et al.*, 2020
Rubberized Concrete	Multi Linear Regression	0.74	Abdollahzadeh *et al.*, 2011

Table 2-8: Coefficient of determination of compressive strength prediction using genetic programming

Concrete	ML technique	R^2	References
HPC	Gene Expression Programming	0.8290	Mousavi *et al.*, 2012
HPC	Genetic Algorithm	0.928	Lim *et al.*, 2004
Envr. friendly concrete	Additive Regression Ensemble GP based	0.9837	Omran *et al.*, 2016
	Bagging Ensemble GP based	0.9815	
Cellular Concrete	Genetic Programming	0.763	Kiani *et al.*, 2016

Table 2-9: Coefficient of determination of compressive strength prediction using SVM models

Concrete	ML technique	R^2	References
HPC	Evolutionary Fuzzy Support Vector Machine Inference Model for Time Series Data	0.9145	M.-Y. Cheng *et al.*, 2012
HPC	Support Vector Machine	0.7798	Rguig and El Aroussi, 2017
	Weighted Support Vector Machine	0.9204	
HPC	Enhanced Cat Swarm Optimization - Support Vector Machine	0.8082	Yu *et al.*, 2018
HPC	Support Vector Machine	0.9913	Gupta, 2006
Cellular concrete	Support Vector Regression (Radial Basis Function)	0.922	Ashrafian *et al.*, 2020
	Support Vector Regression (Polynomial)	0.749	

Table 2-10: Coefficient of determination of compressive strength prediction using ANN models

Concrete	R^2	References	Concrete	R^2	References
HPC	0.9391	M.-Y. Cheng *et al.*, 2012	HPC	0.9030	I C Yeh, 1999
Fly ash concrete	0.9981	Topcu and Saridemir, 2008	Fly Ash and Slag Concrete	0.9065	I C Yeh, 2003
RAC	0.9495	Abdon Dantas *et al.*, 2013	HPC	0.9962	Chithra *et al.*, 2016
Envr. friendly concrete	0.8740	Naderpour *et al.*, 2018	HPC	0.7798	Rguig and El Aroussi, 2017
RAC	0.9968	Duan *et al*., 2013	Conventional concrete and HPC	0.9025	Bui *et al.*, 2018
RAC	0.8670	Deshpande *et al.*, 2014	HPC	0.9722	Yu *et al.*, 2018
RAC	0.9081	Deshpande *et al*., 2016	RAC	0.9987	Ilker Bekir Topçu and Saridemir, 2008
Fly ash and conventional concrete	0.8771	Chopra *et al.*, 2015	Autoclaved aerated concrete	0.9991	Topcu and Saridemir, 2007
HPC	0.6147	Kasperkiewicz *et al.*, 1995	Envr. friendly concrete	0.9590	Omran *et al*., 2016
HPC	0.9991	Oztas *et al.*, 2006		0.9799	
HPC	0.9079	I C Yeh, 1998		0.9702	
SCC	0.9200	Eskandari *et al.*, 2009	SCC	0.9350	Uysal and Tanyildzi, 2011
HPC	0.9100		SCC	0.9024	Siddique *et al.*, 2011
HPC	0.9500	Khan, 2012	Cellular Concrete	0.9345	Ashrafian *et al.*, 2020
HPC	0.8952	Chou and Pham, 2013	UHPC	0.991	Choudhary, 2019
HPC	0.9131	Erdal *et al.*, 2013	Rubberized Concrete	0.9715	Abdollahzadeh *et al.*, 2011

Table 2-11: Coefficient of determination of compressive strength prediction using fuzzy logic models

Concrete	R^2	References
Fly ash concrete	0.9988	Topcu and Saridemir, 2008
RAC	0.9006	Deshpande *et al.*, 2016
RAC	0.9970	Ilker Bekir Topçu and Saridemir, 2008

Table 2-12:Coefficient of determination of compressive strength prediction using other types of models

Concrete	ML technique	R^2	References
Envr. friendly concrete	Gaussian Processes Regression	0.9843	Omran *et al.*, 2016
	Additive Regression Ensemble SMOreg based	0.9681	
	Bagging Ensemble SMOreg based	0.9692	
	Sequential Minimal Optimization Regression	0.9649	
	M5	0.9477	
	Additive Regression Ensemble Decision Stump based	0.9432	
	Bagging Ensemble Decision Stump based	0.8876	
	Decision Stump	0.3854	
Cellular concrete	Standard Multivariate Adaptive Regression Splines	0.9485	Ashrafian *et al.*, 2020
	Multivariate Adaptive Regression Splines with Water Cycle Algorithm	0.973	

Table 2-13: Coefficient of determination of compressive strength prediction using tree-based models

Concrete type	ML technique	R^2	References
RAC	Classification and Regression Tree	0.6959	Deshpande *et al.*, 2014
HPC	Decision Tree	0.8179	Erdal, 2013
	Bagging Decision Tree	0.8787	
	Gradient Boosting Decision Tree	0.8894	
	Random Sub-Spaces Decision Tree	0.8697	
	Two Level Bagging Decision Tree	0.8919	
	Two Level Gradient Boosting Decision Tree	0.9016	
	Two Level Random Sub-Spaces Decision Tree	0.8563	
	Bagging - Random Sub-Spaces Decision Tree	0.8882	
	Random Sub-Spaces - Bagging Decision Tree	0.8903	
	Gradient Boosting - Random Sub-Spaces Decision Tree	0.9224	
	Random Sub-Spaces - Gradient Boosting Decision Tree	0.9086	
CC and HPC	M5P Model Tree	0.9055	Behnood *et al.*, 2017
HPC	M5P Model Tree	0.9505	Yu *et al.*, 2018
Envr. friendly concrete	Additive Regression Ensemble REPTree based	0.9647	Omran *et al.*, 2016
	Bagging Ensemble REPTree based	0.9411	
	REPTree	0.9218	

2.5 Conclusions

This chapter systematically reviewed recent advances in the application of machine learning techniques to predict the compressive strength of non-conventional concretes, including high-performance concrete, self-consolidating concrete, recycled aggregate concrete, FRP-confined concrete, cellular concrete, and engineering cementitious composites. The highly non-linear relationships between the mixture components and the compressive strength of such concretes had necessitated deploying data-driven and intelligent methods for predicting compressive strength. From the critical survey and analysis performed in this chapter, several conclusions can be drawn:

- In general, ML models have proven to be successful in predicting the compressive strength of modern concretes.
- The most commonly applied technique to predict compressive strength is ANN, which has been demonstrated to give superior accuracy. However, being a "black box" tool with high computational cost in comparison to other ML techniques is clearly a disadvantage of this method.
- Fuzzy logic has comparable performance to ANN, but it requires several parameters to be tuned properly and achieve promising accuracy, making the modeling exercise more complex.
- SVM models indicated fair accuracy of output results. However, they reduce the computational cost compared to that of ANN, which makes them a desirable option.
- Hybrid models are powerful tools to overcome the reliance on the hyperparameters tuning of ML techniques since they employ a second model to determine the appropriate hyperparameters for the main model. Thus, such methods seem most promising in future studies and deserve further investigation.
- ML applications are expected to become more prevalent as we are at a time when the internet of things, big data, and automated systems will govern the industrial world in the coming decades.

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Chapter 3

3 Mixture Optimization of Recycled Aggregate Concrete Using Hybrid Machine Learning Model

The scarcity of raw materials, the depletion of landfills, and the footprint caused by the extraction of natural aggregates (NAs) are global environmental concerns regarding to the production of concrete as most widely used construction material. The versatility of concrete along with its vast application worldwide has led to high consumption of its components such as cement, aggregates, etc. The global NA consumption is estimated to be 8 to 12 billion tons annually (Naderpour et al., 2018). This is considered as a major warning so as there have been some reports regarding the shortages of NA resources (Z H Duan et al., 2013; Gholampour et al., 2017). Furthermore, extracting 1 ton of NA results in 0.0046 million tons of carbon emission to the environment (Naderpour et al., 2018).

In addition to the concerns about accessible natural resources, there have been significant problems worldwide regarding the available landfill sites to dispose construction and demolition waste (CDW). In Canada, it is estimated that 9 million tons of CDW are produced every year. Consequently, in spite of the vast area of the country, its biggest cities are encountering CDW disposal issues (Yeheyis et al., 2013). Likewise, several reports are forecasting that in Hong Kong the landfills will be overfilled in eight years (Z H Duan et al., 2013). The use of recycled aggregate (RA) offers a potential solution to overcome the drawbacks related to the production of conventional concrete. Among the most promising advantages of recycled aggregate concrete (RAC) are the significant reductions in the carbon emissions and in the disposal of CDW. In general, 75% of construction waste, including concrete and masonry materials, can be reused as RA in concrete production (González-Fonteboa and Martínez-Abella, 2008).

However, the inclusion of RA in concrete has been proved to reduce its compressive strength (Topçu and Saridemir, 2008). Several researchers have been engaged to determine the most influential factors on the compressive strength of RAC (Zhen Hua Duan and Poon, 2014; Pedro et al., 2015; Poon et al., 2004; Silva et al., 2015). The moisture content of RA, the replacement level of the aggregates, and the water-to-cement ratio are found as the mix

design parameters with the highest impact on the compressive strength (Silva et al., 2015). The higher absorption capacity of RA compared to NA along with the weak bond interface between the raw and recycled components of concrete are the major explanations for such parameters to be highly influential on compressive strength (Deshpande et al., 2014; Poon et al., 2004; Xu, Chen, et al., 2019).

Although there have been multiple studies on the mechanical behavior of RAC, there should be more research devoted to the investigation of the effects of certain parameters on the compressive strength such as moisture content and the crushing process of RA (Pedro et al., 2015; Xu, Zhao, et al., 2019). Considering fundamental knowledge gaps in the mechanical, durability, and structural performance of RAC, its application has been limited to the road foundation and non-structural concrete members (Zhen Hua Duan and Poon, 2014; Topçu and Saridemir, 2008). Overall, it is of great necessity either to carry out comprehensive experimental studies or to deploy advanced practical frameworks to promote the utilization of RAC and subsequently, its quality standards.

The lack of understanding of RAC's mechanical behavior has resulted in the implementation of novel modeling techniques, such as machine learning (ML) algorithms, capable of predicting mechanical properties. One major advantage of ML methods is that they can capture the underlying mechanisms despite the lack of information regarding specific parameters such as the crushing method. Generally speaking, ML techniques have been proven to be successful in the prediction of RAC mechanical properties such as modulus of elasticity and compressive strength. (Behnood et al., 2015; Deng et al., 2018; Deshpande et al., 2014; Khademi et al., 2016). Nevertheless, the majority of the research studies in the open literature employed small datasets which has been considered as a noticeable problem in training of ML models. Ultimately, the collection of more reliable data has been regarded as a research significance in the literature such that several studies aimed at deploying larger data to offer a better generalization and robustness of the RAC-ML models.

ML techniques have also been employed for mix design and optimization. Concrete mix design is the process of selecting the appropriate quantitative proportion of concrete

ingredients (Ziolkowski and Niedostatkiewicz, 2019). From a computational point of view, mixture optimization is the process of minimizing a prior defined objective function (Simon, 2003). A common practice on the concrete mix optimization procedures is to consider the cost function as the objective function (Yeh, 2007; Cheng et al., 2014) (Golafshani and Behnood, 2019). Moreover, the current stringent mechanical requirements for concrete should be met along with the optimization process. Hence, in this study, the particle swarm optimization (PSO) algorithm was used to execute the mixture optimization. Subsequently, to assure that the compressive strength was met, the best performed ML model was used to predict the resistance of the RAC.

Accordingly, the present study aims at creating a large and comprehensive experimental dataset from the available studies in the open literature to develop powerful and state-of-the-art ML models to predict compressive strength of RAC. For this purpose, a dataset consisted of 1134 experimental examples of RAC mixture design along with 10 attributes was developed. Moreover, three different novel ML models are utilized, and their performance was compared. Gaussian processes (GP), deep learning (DL) and gradient boosting regression trees (GBRT) techniques are employed for the first time to model the compressive strength of RAC. Eventually, an optimization of the RAC mixture design was performed by coupling a PSO with the best proposed ML model to develop a hybrid powerful model for optimizing RAC mixture composition for different target ranges of compressive strength at 28 days. The superior accuracy of the proposed models should assist various stakeholders in optimal use of recycled concrete in diverse construction applications.

3.1 Related work

Other studies have employed ML to predict the compressive strength of RAC. For instance, Khademi et al. (2016) used three different approaches to model the compressive strength of RAC: artificial neural network (ANN), adaptive neuro-fuzzy inference systems (ANFIS), and multiple linear regression. They used 14 different input parameters, including the dosage of concrete ingredients and non-dimensional parameters, such as water-to-cement ratio and aggregate-to-cement ratio. It was concluded that multiple linear regression might be inaccurate to determine the compressive strength of RAC due to the

highly non-linear relationships between the concrete ingredients and its strength. However, both ANN and ANFIS models proved to be powerful in modeling the compressive strength of RAC, with a coefficient of determination of 0.9185 and 0.9075 for ANN and ANFIS, respectively. Furthermore, Khademi et. al. (2016) performed a sensitivity analysis, in which they concluded that the inclusion of more input features resulted in higher model predictive accuracy. Likewise, Naderpour et al. (2018) developed an ANN model to predict the compressive strength of RAC with a coefficient of determination of 0.829 for the testing dataset. They also performed a sensitivity analysis via the weights of the input features. Accordingly, it was found that water absorption of aggregates and the water-to-total material ratio resulted with the highest importance. In another study, Deng et al. (2018) built a convolutional neural network to predict the compressive strength of RAC. Experimental work was carried out along with the development of the deep learning model. The authors compared the convolutional neural network with a support vector machine and a back propagation neural network concluding that the convolutional neural network has superior capability to predict the compressive strength of RAC. They used the relative error to measure the performance of the models, and thus the error for the convolutional neural network, the back propagation neural network and support vector machine was 3.65, 6.63, and 4.35, respectively. Deshpande et al. (2014) compared three different techniques: ANN, model tree, and non-linear regression. They studied the influence of adding non-dimensional parameters as input features. To accomplish such analysis, they created 10 different models for each algorithm and added a different non-dimensional input feature to the parameters corresponding to the ingredients content. The accuracy of the ANN model was at least 2% higher than that of the other techniques, even when the non-dimensional parameters were considered. Using a larger dataset, Gholampour et al. (2018) predicted the compressive strength and other mechanical properties of RAC employing three types of algorithms, including multivariate adaptive regression splines, M5 model tree, and least squares support vector regression. They created two different models for each algorithm corresponding to the cube compressive strength and the cylinder compressive strength, respectively. For these models, results on 332 cube-specimens and 318 cylinder-specimens were collected from the open literature. It was found that the least squares support vector regression achieved higher performance than the remaining models, with at least 12.6%

better mean absolute percentage error. Z H Duan et al. (2013) proposed using the characteristics of the recycled aggregates as input parameters, including saturated surface dry mass, water absorption and volume fraction of coarse aggregate. They concluded that the inclusion of these features has a positive effect on model accuracy. Moreover, Topçu and Saridemir (2008) found that ANN had better predictive accuracy than of the RAC compressive and splitting tensile strengths than fuzzy logic. The ANN model demonstrated to be a powerful tool to determine the mechanical properties of RAC, achieving a coefficient of determination of 0.9984, and 0.9979 for the prediction of compressive strength and splitting tensile strength, respectively. Dantas et al. (2013) gathered the largest dataset and used an ANN to develop an equation to describe the compressive strength of RAC. Their model included 17 input features, from which, the ratio of recycled concrete, absorption rate of fine recycled aggregate, content of dry aggregate, and finesses modulus of aggregates were the parameters with the highest effect on the compressive strength of RAC. The reported accuracy for the training and testing sets were 0.928, and 0.971, respectively.

In summary, Khademi et al. (2016), Naderpour et al. (2018) , Deng et al. (2018), Deshpande et al. (2014), Gholampour et al. (2018), Z H Duan et al. (2013), Topçu and Saridemir (2008), and Dantas et al. (2013) used 257, 139, 74, 257, 650, 168, 210, and 1178 data points, respectively to predict compressive strength of RAC. In addition to the quality and size of the existing dataset, the advent of new and more powerful ML algorithms has stimulated researchers to explore the ability of state-of-the-art methods to enhance the accuracy and robustness of predictive models. Among various ML techniques to predict the compressive strength of RAC, artificial neural networks (ANNs), and fuzzy logic are the most widely applied methods as summarized in **Table 3-1**.

3.2 Research Significance

As elaborated on above, there have been various studies on the application of traditional ML techniques to predict the compressive strength of RAC. The present study aims at creating a large and more comprehensive dataset and deploy it with state-of-the-art ML techniques that have not yet been explored for RAC in the open literature. The models presented herein will be executed using Python programming language. Therefore, to

utilize these models, the user can simply apply the development steps along with hyperparameters reported in this study. Furthermore, the compressive strength predictive tools developed in this study are further complemented with optimization in of the mixture proportions using a coupled PSO-GBRT model. The proposed mixture proportions can be used as a reference guideline for designing eco-friendlier and more economical RAC mixtures in practice.

Table 3-1: Studies on using ML techniques for prediction of RAC compressive strength

Machine Learning Technique	No. of samples	References
Artificial neural networks, adaptive neuro-fuzzy inference system and multiple linear regression	257	Khademi *et al.*, 2016
Artificial neural networks	168	Z H Duan *et al.*, 2013
Artificial neural networks, model tree and non-linear regression model	257	Deshpande *et al.*, 2014
Artificial neural networks and fuzzy logic	210	Topçu and Saridemir, 2008
Convolutional neural networks	74	Deng *et al.*, 2018
Artificial neural networks	139	Naderpour *et al.*, 2018
Artificial neural networks	1178	Dantas *et al.*, 2013
Multivariate adaptive regression splines, M5 model tree and least support vector regression	650	Gholampour *et al.*, 2018

3.3 Machine Learning Basis

ML refers to the computers capacity of analyzing data and learning complex patterns within the data without being rigorously programmed (Salehi and Burgueño, 2018). Depending on the nature of the data, ML algorithms are categorized in supervised learning, unsupervised learning and reinforcement learning (Mahdavinejad et al., 2018). Supervised learning aims at capturing underlying patterns in data with known outputs. Depending on the type of the output it further categorized as classification for discrete outputs, and regression for continuous outputs. Unsupervised learning, on the other hand, is associated with the data with unknown outputs and thus, clusters the data by finding relationships within the observations (Murphy, 2012). The third type of machine learning, reinforcement learning, bridges the gap between supervised and unsupervised learning since it clusters similar data given the correct answers (Marsland, 2015). Three powerful ML models were developed herein to forecast the compressive strength of RAC: GP, recurrent neural networks (RNNs), and gradient boosting regression trees (GBRT). The three algorithms

have different approaches for data analysis. Whilst GBRT is an ensemble of decision trees, GP uses the gaussian distribution and finally, RNNs are an advanced type of neural networks. The diverse nature of these algorithms is considered to explore the robustness of ML algorithms. The fundamentals of GP, RNNs, and GBRT are discussed below.

3.3.1 Gaussian Processes

Gaussian processes (GP) are stochastic processes that generalize the Gaussian probability distribution (Noori et al., 2019). In contrast to single- or multi-variable probability distribution in which a scalar or a vector is mapped, a process describes the properties of functions (Rasmussen and Williams, 2006). Therefore, a GP is defined as a probability distribution of functions, P(f), where P(f) has a Gaussian distribution (Omran et al., 2016). GPs are parametrized with mean and covariance by the analogy with Gaussian distribution whereas mean and covariance for GPs are functions (Lawrence, 2005). The purpose of training a supervised learning algorithm using the available training dataset is to develop a model capable of predicting unseen data. In general, there are two common approaches to determine the appropriate function that fits a set of data with promising accuracy (Rasmussen and Williams, 2006). In the first approach, the model is generated by considering only certain types of functions, e.g., exponential functions (Rasmussen and Williams, 2006). However, the prediction accuracy of such models strongly depends on the performance of the given functions. Conversely, the second approach considers pre-assigned probabilities of the several types of functions such that higher probability is assigned to those that are more likely to predict with a higher accuracy (Williams and Barber, 1998). The complexity of the first approach is limited to the selected functions. By contrast, the second approach is not as computationally efficient since there are an infinite number of possible functions to consider (Rasmussen and Williams, 2006). GPs are based on the second approach. The probabilistic formulation of GPs gives rise to a phenomenon called computational tractability in which the properties of the functions are inferred even when some of the functions are ignored (Tobar et al., 2015).

3.3.2 Recurrent Neural Networks

Deep Learning (DL) models are multiple-level computation algorithms able to learn complex underlying structures within a database (Lecun et al., 2015). DL models have been proven to be successful in diverse applications such as image recognition, language understanding, and deoxyribonucleic acid (DNA) biological processes prediction (Lecun et al., 2015). However, the application of recent DL algorithms in civil engineering, including convolutional neural networks (CNNs) and recurrent neural networks have been more common in structural health monitoring and crack detection due to the large data sets available in these fields (Toh and Park, 2020; Ye et al., 2019). CNNs and RNNs are among the most popular DL algorithms. In the present study, a novel RNN is deployed to predict the compressive strength of RAC.

RNN is a class of Neural Networks with an internal loop that allows the algorithm to keep memories from past information, commonly referred to as hidden state (Chollet, 2018; Gulli and Pal, 2017). In RNNs, the output of a certain step, t, is used as the input for the next step, t+1, emphasizing that every single step is based on the previous one, a process referred to as long-term dependencies; see **Figure 3-1** (Gulli and Pal, 2017). Simple RNNs have a limitation regarding the contribution of earlier steps to the later ones known as vanishing gradients (Gulli and Pal, 2017). Two main variants of layers have been proposed for RNN to overcome vanishing gradients: long short-term memory (LSTM) and gated recurrent unit (GRU) (Chollet, 2018). The main difference of these RNN algorithms relies on the inclusion of gates for computing data. For example, LSTM layers incorporate a third gate, named the forget gate, in addition to the input and output gates in the simple RNN (Gulli and Pal, 2017). The forget gate maintains the information and includes it in a non-consecutive step (Chollet, 2018). Conversely, GRU layers have only two types of gates: reset gate and update gate. In the reset gate, the previous information is combined with the most recent information, whereas in the update gate, it is decided how much information is to be passed to the following step. **Figure 3-2** displays the structure of the first GRU layer used in this study (Gulli and Pal, 2017). Like LSTMs, GRUs are not affected by vanishing gradients. Nonetheless, GRU is considered a more efficient algorithm due to its

simpler structure and formulation (Gulli and Pal, 2017). The formulation of GRU is summarized in the following:

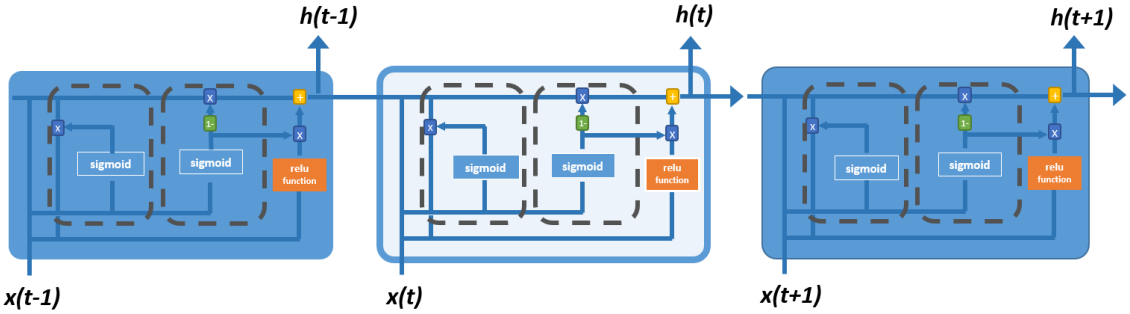

Figure 3-1: RNN structure using one GRU hidden layer.

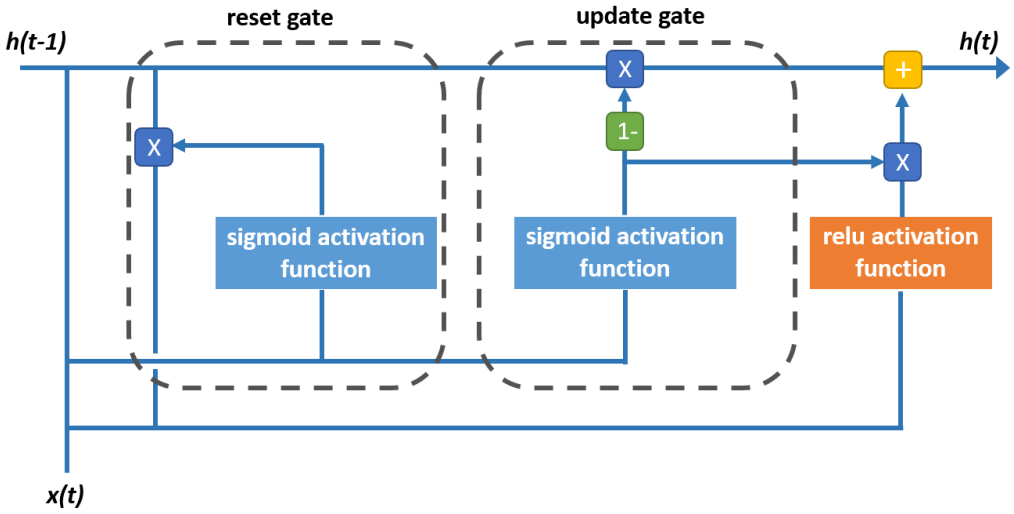

Figure 3-2: GRU hidden state computation, first layer of the developed deep learning model.

$$r_t = \sigma(W_r\, x_t + U_r\, h_{t-1}) \quad \textbf{(3-1)}$$

$$z_t = \sigma(W_z\, x_t + U_z\, h_{t-1}) \quad \textbf{(3-2)}$$

$$\bar{h_t} = ReLu\big(W_h\, x_t + U_h\, (r_t \times h_{t-1})\big) \quad \textbf{(3-3)}$$

$$h_t = (1 - z_t) \times h_{t-1} + z_t \times \bar{h_t} \quad \textbf{(3-4)}$$

where r_t and z_t are the reset and update gate, respectively, $\bar{h_t}$ is the candidate output, and h_t is the corresponding output of the cell for the time step t. Accordingly, $W_r, W_z, W_h, U_r, U_z,$ and U_h are the weight matrices that operate the input vector x_t and the previous state h_{t-1} , and ReLu is the rectified linear unit activation function(Yao et al., 2015; Zhao et al., 2019).

3.3.3 Gradient Boosting Regression Trees

GBRT algorithm integrates multiple weak learners using a boosting approach in which additional trees are appended in sequence without model parameters being changed. The objective of the gradient boosting is to find the function $F(X)$ which minimizes the loss function $L(F(X), Y)$ (e.g. mean squared error or mean absolute error) using a given dataset, $\{(x_1, y_1), (x_2, y_2), \dots, (x_N, y_N)\}$ (J. Friedman, 2001; Zhan *et al.*, 2020). The predictions of GBRT model, y_t for a given input data can be expressed as:

$$y_t = \mathcal{F}_m(\mathcal{X}_t) = \sum_{m=1}^{M} \hbar_m(x_t) \quad \textbf{(3-5)}$$

Where the $\hbar_m$ are referred to as weak learners. The constant M represents the number of weak learners which is known as the `n_estimators` hyperparameter. The loss function represents to what extent the predicted value is close to the output in the dataset using a specific metric. GBRT approaches the best function using the weighting of weak learner models, $h(x_t)$, which is the basic decision tree fit by the input variables and the negative gradient of the last model's loss function. GBRT develops the model in a greedy manner considering a constant initial function $F_0(X)$ as follows (J. Friedman, 2001; J.H. Friedman, 2002; Persson *et al.*, 2017; Zhan *et al.*, 2020):

$$F_0(X) = argmin \sum_{t=1}^{N} \mathcal{L}(y_t, \gamma) \quad \textbf{(3-6)}$$

$$\mathcal{F}_m(\mathcal{X}) = \mathcal{F}_{m-1}(\mathcal{X}) + \gamma_m \hbar_m(x) \quad \textbf{(3-7)}$$

Where $\hbar_m(x)$ is the mth regression tree and γ_m is its weighting coefficient, also called learning rate. In a GBRT model, the number of trees, the learning rate, and the max depth of the tree are amongst the most essential hyperparameters that noticeably affect the predictive performance of the model. Larger number of trees increases the prediction

accuracy of the model; however, excessive trees could result in an over-fitted model with lack of generalization for new unseen data. On the other hand, the learning rate controls the contribution of each tree to the predictions, while the max depth indicates the complexity of each tree. Immoderate values of such hyperparameters could bring about either over-fitted or erroneous models (J. Friedman, 2001; J.H. Friedman, 2002; Persson *et al.*, 2017; Zhan *et al.*, 2020). Other parameters of the GBRT model, such as subsample, maximum number of features, etc., also have noticeable effects on the model output and should be considered. Hence, tuning the GBRT hyperparameters is essential to propound robust and reliable performance.

3.4 Dataset Creation and Model Development

3.4.1 Data Collection and Preprocessing

The experimental data used in this dissertation was collected from 55 peer-reviewed publications (**Table 3-2**). The collected data consists of 1134 recycled aggregate concrete mixture design examples, with 9 input features and one output. Statistical characteristics of the dataset are given in **Table 3-3**. **Figure 3-3** illustrates the Pearson correlation coefficient between different attributes of the dataset. The Pearson correlation coefficient is an indicator of linear dependencies within two random variables; *i.e.*, a coefficient of correlation close to one within two variables indicates that an increase in one of those variables will result in a proportional increment of the other (Benesty et al., 2009). Accordingly, the water-to-cement ratio and superplasticizer dosage were the features having highest correlation to the compressive strength. Conversely, aggregates (sand, natural gravel and recycled coarse aggregate), did not have significant linear correlation to the compressive strength. Furthermore, since gravel is an ingredient replaced by recycled coarse aggregate (RCA), there was a high correlation between these two features.

Table 3-2: Sources of experimental data used in this thesis

Reference	No. of Samples	Reference	No. of Sample
M. C. Limbachiya *et al.*, 2000	12	Manzi *et al.*, 2013	10
A. Ajdukiewicz and A. Kliszczewicz, 2002	117	A. B. Ajdukiewicz and A. T. Kliszczewicz, 2017	16
Gómez-Soberón, 2002	15	Sheen *et al.*, 2013	27
Y. H. Lin *et al.*, 2004	24	Thomas *et al.*, 2013	72
C. S. Poon *et al.*, 2004	36	Ulloa *et al.*, 2013	18
D. Matias *et al.*, 2013	9	Taffese, 2018	10
Etxeberria, Marí *et al.*, 2007	4	Andreu and Miren, 2014	30
Etxeberria, Vázquez *et al.*, 2007	12	Beltrán, Agrela, *et al.*, 2014	9
Kou *et al.*, 2007	40	Beltrán, Barbudo, *et al.*, 2014	8
Poon *et al.*, 2007	8	Çakır and Sofyanlı, 2015	27
Rahal, 2007	70	Carneiro *et al.*, 2014	2
Sato *et al.*, 2007	11	Dilbas *et al.*, 2014	12
Casuccio *et al.*, 2008	9	Zen Hua Duan and Poon, 2014	26
Kou *et al.*, 2008	24	Folino and Xargay, 2014	4
Yang *et al.*, 2008	42	López Gayarre *et al.*, 2014	14
Domingo-Cabo *et al.*, 2009	8	Medina *et al.*, 2014	16
Corinaldesi, 2010	10	Pedro *et al.*, 2015	18
Kumutha and Vijai, 2010	12	Pepe *et al.*, 2014	15
Malešev *et al.*, 2010	9	Wardeh *et al.*, 2015	16
Belén *et al.*, 2011	16	Haitao and Shizhu, 2015	20
Fathifazl *et al.*, 2011	6	Tam *et al.*, 2015	24
Chakradhara Rao *et al.*, 2011	16	Abdel-Hay, 2017	4
Somna *et al.*, 2012	18	Zheng *et al.*, 2018	36
Abd Elhakam *et al.*, 2012	30	Nepomuceno *et al.*, 2018	15
Barbudo *et al.*, 2013	36	Mohammed *et al.*, 2018	12
Butler *et al.*, 2013	8	Thomas *et al.*, 2018	23
Ismail and Ramli, 2013	12	Younis and Pilakoutas, 2013	18
Kim *et al.*, 2013	18		

Feature normalization is a commonly applied preprocessing technique prior to modeling. Although normalization is not required for all machine learning algorithms, it has been proven to improve the model performance (Marsland, 2015). Linear transformation and statistical standardization are among the most popular normalization techniques (Shanker et al., 1996). In the linear transformation, values are ranged within a domain of [0,1], whereas in the statistical standardization, the mean and the standard deviation values of the data are set equal to 0 and 1, respectively (Shanker et al., 1996). In this study, statistical

standardization was used prior to GP and recurrent neural networks (RNNs) modeling. The data was then randomly divided into training and testing sets using 70% (793 samples) for training and the remaining (341 samples) for testing.

Table 3-3: Statistical characteristics of the dataset

Input feature	Units	Min.	Max.	Mean	Standard deviation
Water-to-cement ratio	-	0.237	1.020	0.492	0.117
Cement content	kg/m^3	210.00	650.00	387.601	71.358
Sand content	kg/m^3	419.52	1010.00	691.711	131.652
Recycled aggregate content	kg/m^3	0.00	1358.00	527.829	444.749
Gavel content	kg/m^3	0.00	1524.00	542.945	470.187
Superplasticizer	kg/m^3	0.00	45	2.634	4.526
Silica fume content	kg/m^3	0.00	50.00	3.472	11.593
Age	Days	2.00	365.00	44.572	70.692
Specimen type	Type	1.00	5.00	2.786	1.148
Output	**Units**	**Min**	**Max**	**Mean**	**Standard deviation**
Compressive strength	MPa	4.300	108.510	43.567	17.720

A common practice to assess the performance of ML models is to divide the whole set into three different subsets: training, validation and testing. Whilst the learning process is accomplished with the training set, the validation set is used to track the performance of the model, while the testing set serves to assess the extrapolation capabilities of the model by performing it over unseen samples (Marsland, 2015). However, the partition of data into three subsets leads to a reduction of the training samples which consequently might end in an insufficiently trained model (Marsland, 2015). Thus, cross validation is a common technique to prevent the over reduction of the training set, especially for small datasets. There are several techniques to perform cross validation, most of which consist in leaving out random data to validate the model (Nilsen et al., 2019). In this study, K-fold cross-validation was utilized. K-fold cross-validation is a resampling method that splits the data into K number of subsets and keeps one subset for validation, while the other k-1 subsets are used for training (Hastie et al., 2008). The 5-fold cross-validation employed for hyperparameter selection in this study is schematically depicted in **Fig. 4**.

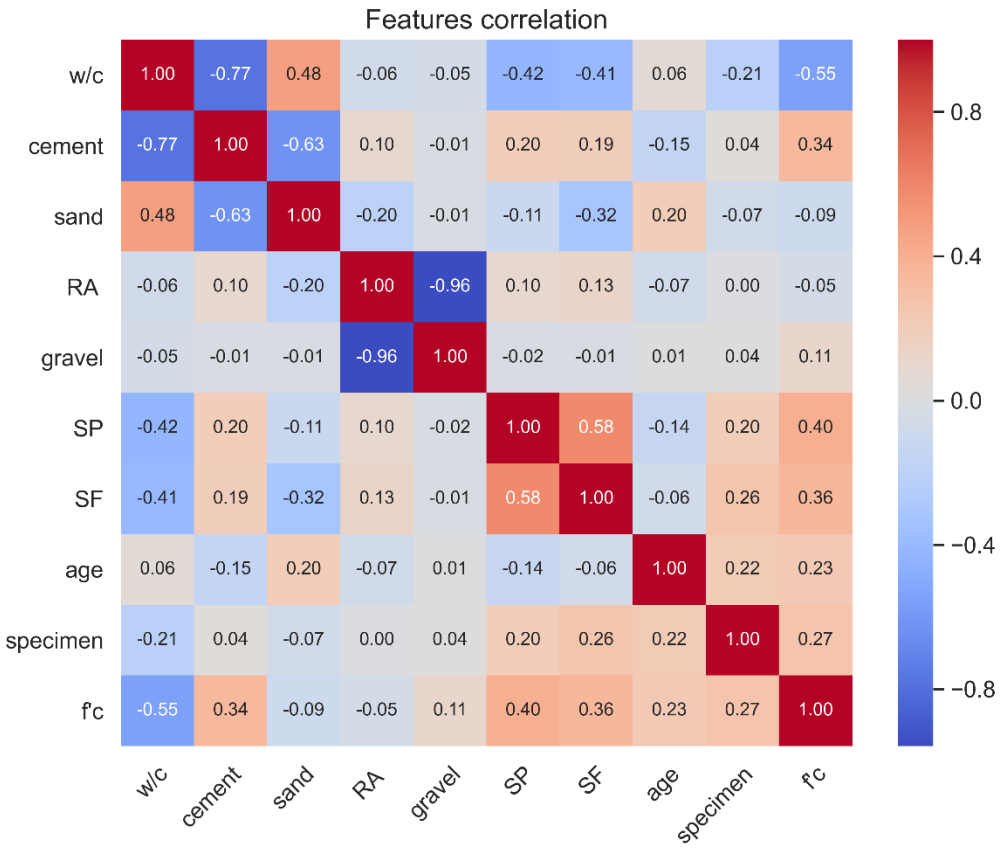

Figure 3-3: Pearson correlation coefficient for the dataset attributes.

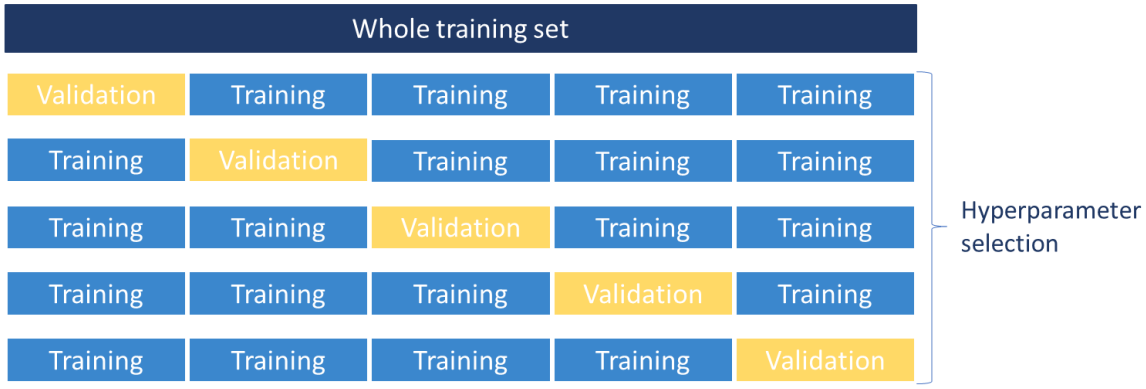

Figure 3-4: 5-fold cross validation for hyperparameter tuning.

3.4.2 Hyperparameter Tuning

Hyperparameter tuning is a crucial step in developing robust ML models. Tuning of the ML model would mitigate the over-fitting and thus, enhance the versatility of the model to

unseen data (Bardenet et al., 2013). The selection of optimum hyperparameters is also a determinant factor in increasing the model accuracy (J. Bergstra et al., 2013). Aiming to avoid manual tuning, there have been different approaches proposed to automize the selection of hyperparameters such as grid search and random search hyperparameter optimization (James Bergstra and Bengio, 2012). These approaches are distinguished from each other by the domain of the potential values considered in the search attempt. Whilst grid search explores all possible values in a pre-defined domain for hyperparameters, random search algorithms select the different hyperparameter values in a random manner for a specific number of iterations (James Bergstra and Bengio, 2012). In this study, a randomized search procedure along with a 5-fold cross validation were used for the exploration of possible values for hyperparameters using the `Scikit-learn` package in python (Varoquaux *et al.*, 2015).

3.4.3 Model Development

3.4.3.1 GP Model

GP is a non-parametric model (Rasmussen and Williams, 2006) and thus, the selection of hyperparameters is less challenging, especially compared to DL models. The hyperparameters of GP models are those required for the kernel function. Therefore, the kernel function, also known as the covariance function, is key to creating robust GP models (Rasmussen and Williams, 2006). In this thesis, a linear combination of several default kernel functions was implemented as defined in **Eq. 3-8**. This kernel function includes the periodic kernel, Matérn kernel, and dot-product kernel. It is worth mentioning that all available kernels, such as the periodic kernel, the rational quadratic kernel, white kernel, Matérn kernel, and dot-product kernel, were tested for tuning the GP model.

$$k(x_i, x_j) = \sigma_0^2 + x_i \cdot x_j + 2^2 * \exp\left(-\frac{2\ sin^2\left(\pi\frac{d(x_i,x_j)}{p}\right)}{l_1^2}\right) + \frac{1}{\Gamma(\nu)2^{\nu-1}}\left(\frac{\sqrt{2\nu}}{l_2}\ d(x_i,x_j)\right)^{\nu} K_\nu\left(\frac{\sqrt{2\nu}}{l_2}\ d(x_i,x_j)\right) \quad \textbf{(3-8)}$$

According to the former equation, parameters associated with the considered kernels were tuned as the hyperparametrs of the GP model, including the length scale 1 (l_1) and periodicity (p) corresponding to the periodic kernel; ν and length scale 2 (l_2) corresponding to the matern kernel; and σ_0 of the dot-product kernel. The optimizing of hyperparameters

was carried out using 5-fold cross-validation (CV) as described earlier. The tuned values of the hyperparameters are listed in **Table 3-4.** `Scikit-learn` library in Python was employed for tuning and executing the GP model (Varoquaux *et al.*, 2015).

Table 3-4: Hyperparameters for gaussian processes model

Hyperparameter	Assigned value
Length scale 1, l_1	0.6
Periodicity, p	16.0
Sigma naught, σ_0	1.9
Length scale 2, l_2	1
Nu, ν	0.5

3.4.3.2 RNN Model

The developed architecture of the RNN model consists of 3-GRU layers and 1 dense layer having 239, 238, 217, and 1 hidden neuron, respectively. In the first layer, rectified linear unit (ReLU) activation function and sigmoid recurrent activation function were utilized (**Figure 3-2**). In the second layer, the activation function and the recurrent activation function were sigmoid and ReLU, respectively. In the third layer, scaled exponential linear unit (SELU) and softsign were used as activation and recurrent activation functions, respectively. For the dense layer, only softplus activation function was used. Moreover, the kernel initializer and recurrent initializer were tuned for GRU layers. The kernel initializer was fixed as random uniform for first and second layer, whereas constant initializer was used for the third layer. The recurrent initializer was set as constant for the first layer, and zeros recurrent initializer for the second and third layer. Mean squared error (MSE) was used as the model loss function, whereas the Adam optimization algorithm was employed as the model optimizer, with a learning rate of 0.0002. Ultimately, the number of epochs and batch size was set to 360 and 11, respectively. According to Whang and Matsukawa (Whang and Matsukawa, n.d.), the performance of GRU models is improved when batch normalization is applied. Batch normalization mitigates the so-called internal covariate shift (Whang and Matsukawa, n.d.). Internal covariate shift is a frequent problem in the training step of deep neural networks in which the distribution of the inputs at each layer is changed and thus, a finer tuning for models along with smaller learning rates are required (Ioffe and Szegedy, 2015). Hence batch normalization was implemented in the developed

RNN model as it has been proven to improve the performance of GRU networks (Whang and Matsukawa, n.d.). Momentum and epsilon are the parameters associated with the batch normalization. The optimum momentum and epsilon were found to be 0.95 and 0.0001, respectively. **Table 3-5** summarizes the tuned hyperparameters of the RNN model. The hyperparameter selection for the deep learning models was performed using a randomized search approach along with 5-fold CV. `Keras API` and `Scikit-learn` packages in Python were utilized for building and tuning the RNN model (Chollet *et al.*, 2015; Varoquaux *et al.*, 2015).

Table 3-5: Hyperparameters for deep learning model

Layer	Units	Activation function	Recurrent activation function	Kernel initializer	Recurrent initializer
Gated recurrent unit	239	ReLU	Sigmoid	Random Uniform	Constant
Gated recurrent unit	238	Sigmoid	ReLU	Random Uniform	Zeros
Gated recurrent unit	217	SELU	Softsign	Constant	Zeros
Dense	1	Softplus	-	-	-

3.4.3.3 GBRT Model

GBRT has multiple hyperparameters that need tuning prior to model training. In the current thesis, a randomized search procedure alongside 5-fold CV was used to obtain optimum hyperparameters of the GBRT model. Generally, `n_estimators` and `learning_rate`, which indicate the number of the weak learners in the model and the weighting of each estimator, respectively, are the most influential hyperparameters of the GBRT model that are essential to be tuned. Additionally, `max_depth`, `max_features`, and `subsample` can greatly affect the prediction performance of the GBRT model (Marani and Nehdi, 2020). **Table 3-6** presents the tuned values of the 7 hyperparameters considered. The mean absolute error (MAE) was monitored as the statistical error to achieve optimum hyperparameters yielding highest accuracy while mitigating over-fitting. The `Scikit-learn` package was implemented to perform GBRT modeling and tuning (Varoquaux et al., 2015).

Table 3-6: Hyperparameters for GBRT model

Hyperparameter	Number of estimators	Learning rate	Min samples split	Min samples leaf	Max depth	Max features	Subsample
Value	315	0.44	33	17	5	7	0.98

3.4.3.4 RCA Mixture Optimization

This section presents the framework adopted for optimizing the mixture design of RAC using the ML model with best predictive performance. The objective of the optimization is to propose the most economic mixture proportions of RAC considering different classes of compressive strength. The PSO algorithm, which is a metaheuristic method which mimics the social interactions of birds or insects (particles) in the search of an optimal solution, was adopted (Penadés-Plà et al., 2016). The particles modify their position in every iteration based on the individual velocity vector of each particle which in turn is dependent on the both best found particle and swarm positions (Lu et al., 2012). The PSO minimizes an objective function while limiting the domain for the solution. According to the optimization procedure proposed by Yeh (Yeh, 2007), the function that is to be optimized herein is the cost to produce a batch of RAC as defined in **Eq. 3-9**. The considered unit costs, which are averages of values retrieved from multiple material suppliers across Canada, are presented in **Table 3-7**. These values can easily be replaced by cost corresponding to other locations. The unit cost of RCA was considered equal to that of NA as recommended in ref. (Wijayasundara et al., 2016).

$$P = C_1 I_1 + C_2 I_2 + \cdots + C_i I_i \quad \textbf{(3-9)}$$

Table 3-7: Unit price of ingredients of concrete mixtures

Ingredient	Units	Currency	Unit price
Water	$/kg	Canadian dollar	0.004
Cement	$/kg	Canadian dollar	0.43
Sand	$/kg	Canadian dollar	0.28
Recycled aggregate	$/kg	Canadian dollar	0.20
Gavel	$/kg	Canadian dollar	0.20
Superplasticizer	$/kg	Canadian dollar	71.07
Silica fume	$/kg	Canadian dollar	2.85

were C_i represents the unit cost of the ith ingredient of the mixture and I_i is the i^{th} ingredient dosage in kg/m^3. To limit the domain of the solution, two bounder vectors were defined: upper limit and lower limit. The bounder vectors (**Table 3-8**) were strategically defined based on a real experiment from the dataset with certain compressive strength to draw a meaningful comparison and thus, better validate the performance of the algorithm. In other words, for sand, cement, and water, the upper and lower bounder limits were defined in average 20% up and down the values given for the base mixture. To promote the use of recycled aggregate, the assigned values to the lower and upper bounder vectors were kept high, and the corresponding values for gravel were maintained low. Also, due to the high cost of superplasticizer, the assigned values for the bounder vectors were kept as low as possible. The 28-days compressive strength of a standard $15x30\ cm$ cylinder specimen was considered for sake of comparison. The results of the optimized mixture proportions are given in **Table 3-9**. The optimized mixture was tested using the GBRT (being the best predictive model in this study) and compared to the real concrete sample extracted from the dataset to ensure the required compressive strength criteria as shown in **Table 3-10**.

Table 3-8: Bounder vectors for mixture optimization

Input feature	Unit	25 MPa		30 MPa		35 MPa		40 MPa		45 MPa	
		Upper limit	Lower limit	Upper limit	Lower limit	Upper limit	Lower limit	Upper limit	Lower limit	Upper limit	Lower limit
Water	kg/m³	350	200	350	190	230	160	230	160	200	140
Cement	kg/m³	424	290	424	292	424	323	424	280	450	300
Sand	kg/m³	942	650	942	650	942	720	942	750	950	800
RA[a]	kg/m³	1080	700	1080	750	1080	550	900	750	500	50
Gavel	kg/m³	511	50	511	50	511	100	750	220	1080	700
SP[b]	kg/m³	0	0	0	0	0	0	2	0.9	2	0
Age	Days	28	28	28	28	28	28	28	28	28	28
Specimen	Type	1	1	1	1	1	1	1	1	1	1

[a] recycled aggregate [b] superplasticizer

Table 3-9: Optimized mixtures

Optimized Mix	Water	Cement	Sand	RA[a]	Gravel	SP[b]	Age	ST[c]
	[kg/m³]	[kg/m³]	[kg/m³]	[kg/m³]	[kg/m³]	[kg/m³]	Days	Type
25 MPa	246.46	296.62	701.67	711.90	155.23	0.00	28	1
30 MPa	239.56	298.52	701.67	760.33	155.23	0.00	28	1
35 MPa	181.68	327.99	759.29	566.60	193.82	0.00	28	1
40 MPa	178.83	310.45	767.23	768.92	313.78	1.23	28	1
45 MPa	154.43	354.75	804.17	63.74	816.17	0.24	28	1

[a] recycled aggregate [b] superplasticizer [c] specimen type

Table 3-10: Comparison of optimized mixture with base mixture

Input feature	Units	25 MPa		30 MPa		35 MPa		40 MPa		45 MPa	
		Base	Opt.	Base	Opt.	Base	Opt.	Base	Opt.	Base	Opt.
Water	kg/m³	234.10	246.46	190.00	239.56	175.00	181.68	187.00	178.83	219.75	154.43
Cement	kg/m³	390.16	296.62	380.00	298.52	350.00	327.99	311.00	310.45	323.08	354.75
Sand	kg/m³	702.30	701.67	637.00	701.67	730.00	759.29	840.00	767.23	948.92	804.17
RA[a]	kg/m³	1053.45	711.90	1123.00	760.33	989.00	566.60	0.00	768.92	259.39	63.74
Gravel	kg/m³	0.00	155.23	0.00	155.23	0.00	193.82	935.00	313.78	771.00	816.17
SP[b]	kg/m³	0.00	0.00	0.00	0.00	1.68	0.00	1.56	1.23	0.00	0.24
Age	Days	28	28	28	28	28	28	28	28	28	28
ST[c]	Type	1	1	1	1	1	1	1	1	1	1
f'c	**MPa**	**25.3**	**25.5**	**30.1**	**29.6**	**36.0**	**35.5**	**40.0**	**39.9**	**45.6**	**44.7**
Price	**CAD**	**577.21**	**499.44**	**568.49**	**510.02**	**673.94**	**507.12**	**668.66**	**654.35**	**612.85**	**572.19**

[a] recycled aggregate [b] superplasticizer [c] specimen type

3.5 Results, Discussion and Recommendations

This section presents the results of ML modeling of RAC. The three different models outlined earlier were implemented and their prediction performance is discussed herein. Purposefully, the root mean squared error ($RMSE$), mean absolute error (MAE), and coefficient of determination (R^2) are monitored for assessing the performance of each model. Moreover, the best acquired ML model was employed to perform RAC mixture design optimization for different ranges of 28-day compressive strength. The optimization results along with mixture proportion recommendations are discussed below.

3.5.1 Prediction Performance of ML Models

GP, GRU, and GBRT models were trained using 793 training data and tested with the remaining 341 data. The final tuned models were executed over five different seed numbers of data split to assess the robustness of the models trained with randomized split of the data for training and the testing sets. The predictive performance of the GP model for five random seed numbers is summarized in **Table 3-11**. The model predicted the output with an average $RMSE$, MAE and R^2 of 7.087 MPa, 4.911 MPa, and 0.844, respectively for the test dataset. However, the model performance was greatly superior for the training dataset with average $RMSE$, MAE and R^2 of 0.735, 0.138, and 0.998, respectively. This trend can be further observed in the residual plot of the GP model shown in **Figure 3-5**. The residuals for the training data were less than 10 MPa, while they were as high as 40 MPa for some data points in the testing set. The actual versus predicted output of the GP model is illustrated in **Figure 3-6**.

Table 3-11: Measured performance of gaussian process model

Random Seed and Global Performance	Set	*RMSE*[b]	*MAE*[c]	R^2
RS[a] = 59	Test	7.468	5.157	0.827
	Train	0.556	0.111	0.999
RS[a] = 1718	Test	7.589	5.197	0.834
	Train	0.789	0.144	0.998
RS[a] = 1009	Test	6.582	4.762	0.854
	Train	0.595	0.103	0.999
RS[a] = 3097	Test	7.492	4.875	0.841
	Train	0.680	0.135	0.998
RS[a] = 7	Test	6.305	4.566	0.862
	Train	1.055	0.197	0.997
Average	**Test**	**7.087**	**4.911**	**0.844**
	Train	**0.735**	**0.138**	**0.998**
Standard Dev	**Test**	**0.597**	**0.267**	**0.014**
	Train	**0.200**	**0.037**	**0.001**

[a] random seed [b] root mean squared error [c] mean absolute error

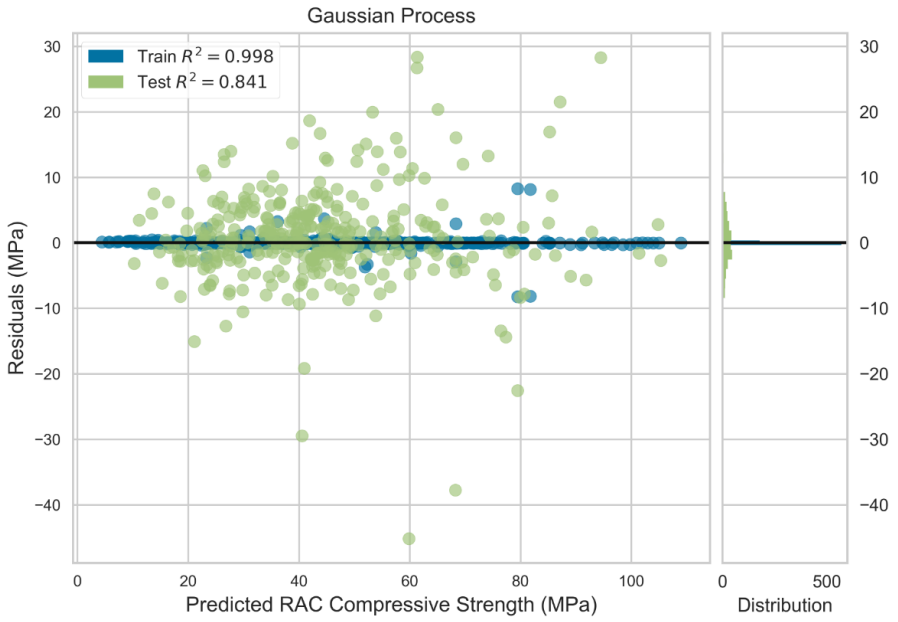

Figure 3-5: Residuals plot for gaussian process model.

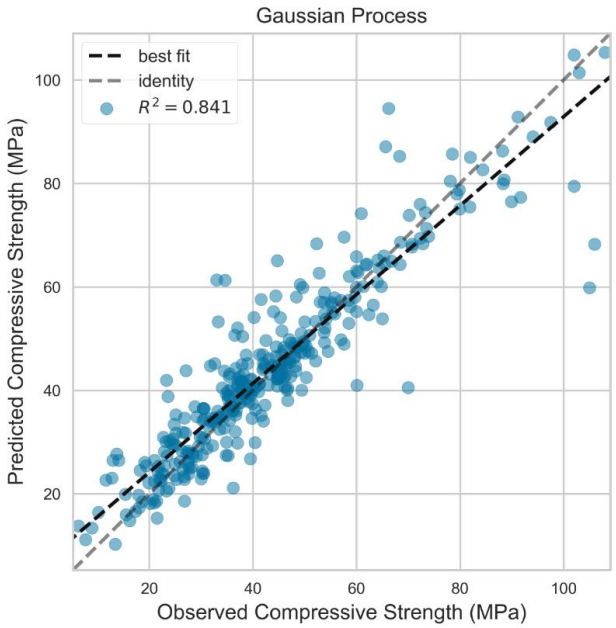

Figure 3-6: Actual vs. predicted values for testing set in Gaussian process model.

The GRU model attained better performance compared to that of the GP model (see **Table 3-12**). The difference between the GRU statistical errors of train and test data were less than that of the GP model. The $RMSE$, MAE and R^2 values for the test dataset were 6.502

MPa, 4.364 MPa, and 0.868, respectively, while the corresponding values were 3.183 MPa, 2.285 MPa, and 0.968, respectively, for the train dataset. This demonstrates more robust predictive performance along with higher accuracy compared to the GP model. The residuals of the predictions varied in a narrower range compared to that in the GP model, as depicted in **Figure 3-7**. The residuals for both testing and training datasets had similar normal distribution, indicating more robust predictive performance. **Figure 3-8** shows the actual versus predicted compressive strength of the test data for the GRU model.

Table 3-12: Measured performance of deep learning model

Random Seed and Global Performance	Set	*RMSE*[b]	*MAE*[c]	R^2
RS[a] = 59	Test	7.298	4.663	0.835
	Train	3.064	2.16	0.97
RS[a] = 1718	Test	6.927	4.567	0.861
	Train	3.140	2.274	0.968
RS[a] = 1009	Test	5.778	4.106	0.888
	Train	3.172	2.316	0.969
RS[a] = 3097	Test	6.589	4.312	0.877
	Train	3.144	2.251	0.967
RS[a] = 7	Test	5.918	4.172	0.878
	Train	3.394	2.422	0.965
Average	**Test**	**6.502**	**4.364**	**0.868**
	Train	**3.183**	**2.285**	**0.968**
Standard Dev	**Test**	**0.649**	**0.243**	**0.021**
	Train	**0.125**	**0.096**	**0.002**

[a] random seed [b] root mean squared error [c] mean absolute error

The GBRT model scored superior predictive execution, as indicated in **Table 3-13**, with lowest $RMSE$ and MAE values for the test data, along with the highest coefficient of determination compared to that of the GP and GRU models. $RMSE$ and MAE were 5.074 and 3.396 MPa, respectively for the GBRT model. **Figure 3-9** depicts the residuals of the predicted compressive strength for the training and testing datasets of the GBRT model. It can be observed that the model captured the trend in the data and demonstrated powerful performance on both the train and test datasets. The model achieved R^2 value of 0.997 and 0.925 for training and testing data, respectively. Furthermore, less scatter of the GBRT predicted values of the test dataset was accomplished compared to the GRU and GP

models. The actual versus GBRT predicted compressive strength of the test data is displayed in **Figure 3-10**.

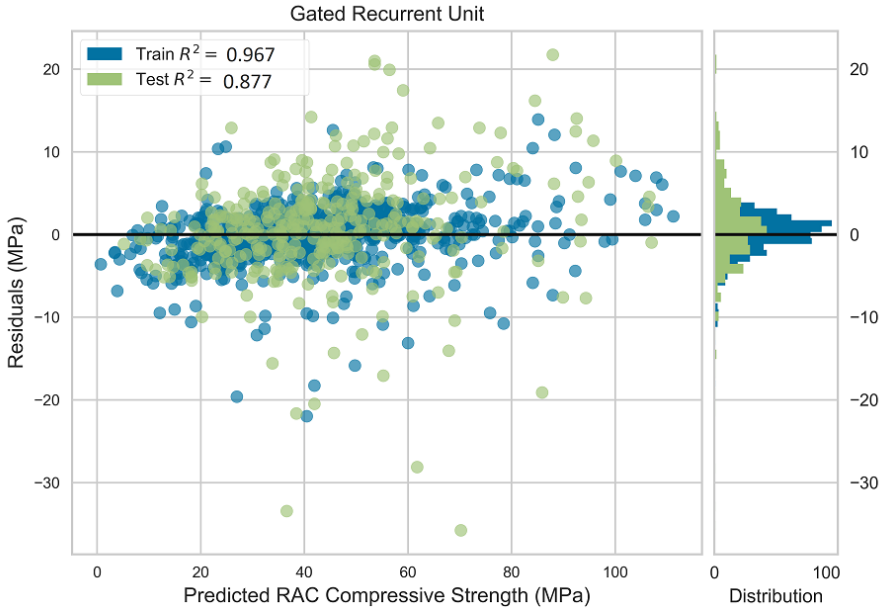

Figure 3-7: Residuals plot for deep learning model.

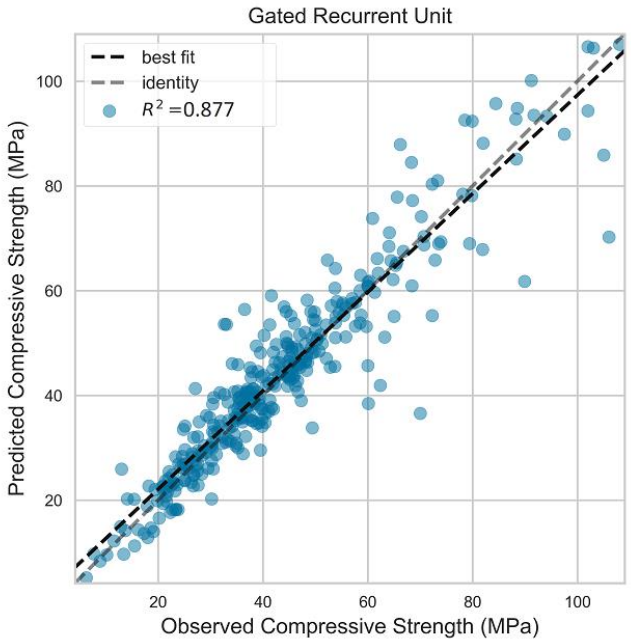

Figure 3-8: Actual vs. predicted values for testing set in deep learning model.

Table 3-13: Measured performance of GBRT model

Random Seed and Global Performance	Set	*RMSE*[b]	*MAE*[c]	R^2
RS[a] = 59	Test	5.124	3.354	0.918
	Train	1.102	0.743	0.996
RS[a] = 1718	Test	5.359	3.698	0.917
	Train	1.008	0.710	0.996
RS[a] = 1009	Test	4.640	3.196	0.927
	Train	0.965	0.683	0.997
RS[a] = 3097	Test	5.168	3.335	0.924
	Train	0.970	0.704	0.996
RS[a] = 7	Test	5.087	3.398	0.911
	Train	1.052	0.748	0.996
Mean	**Test**	**5.076**	**3.396**	**0.919**
	Train	**1.019**	**0.718**	**0.996**
Standard Dev	**Test**	**0.236**	**0.165**	**0.005**
	Train	**0.051**	**0.024**	**0.0003**

[a] random seed [b] root mean squared error [c] mean absolute error

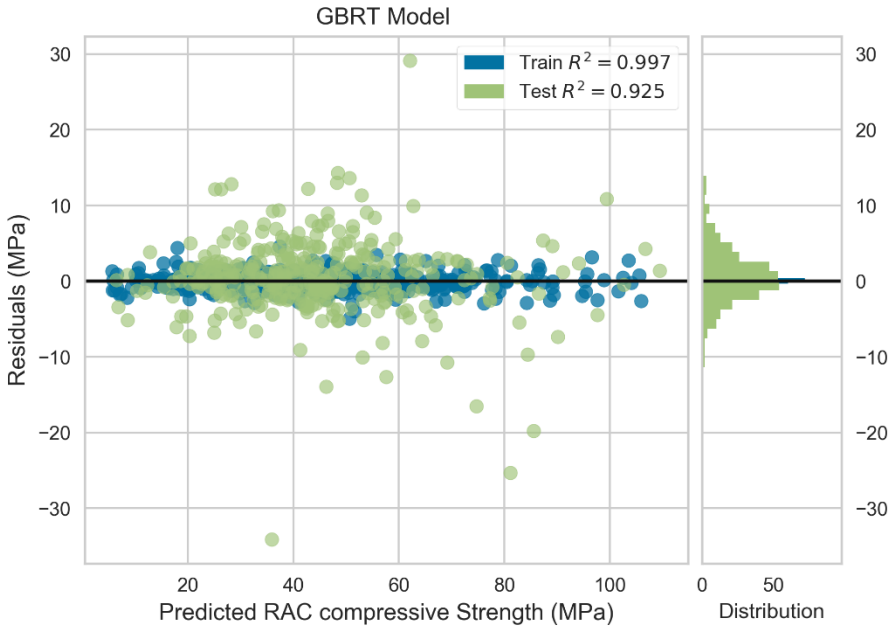

Figure 3-9: Residuals plot for GBRT model.

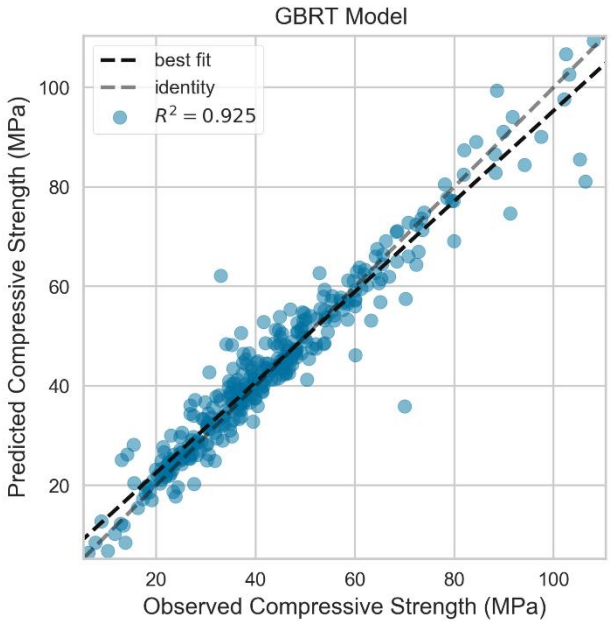

Figure 3-10: Actual vs. predicted values for testing set in GBRT model.

3.5.2 Comparison of Model Performance

Based on the results discussed above, all developed ML models could predict the compressive strength RAC with a reasonable accuracy. However, the GRU and GBRT models demonstrated higher generalization capacity as the prediction errors for training and testing sets were highly analogous in contrast to the GP model. The prediction accuracy for the training set in the GP model was very high while it was quite low for the testing dataset. Thus, the GP model suffers from over-fitting and lack of generalization to new unseen data. Although DL models are recognized to be more accurate on large datasets, the finely tuned GRU model, despite the relatively small dataset, reached outstanding prediction performance with high generalization capacity.

Figure 3-11 illustrates the Taylor diagram of the GP, GRU and GBRT models using the $RMSE$, Pearson correlation and standard deviation of the predictions. The Taylor diagram suggests that the GBRT model had superior performance in terms of $RMSE$, whereas the GRU model provided predictions of the output with a highly correlated standard deviation to the actual observations. It is worth mentioning that the GBRT model required considerably shorter execution time for training compared to the GRU model. This

comparison was performed using the same computer without mounting or connecting it to a hosted GPU. Ultimately, it was concluded that the GBRT model had the best performance and will be considered for the mixture optimization process.

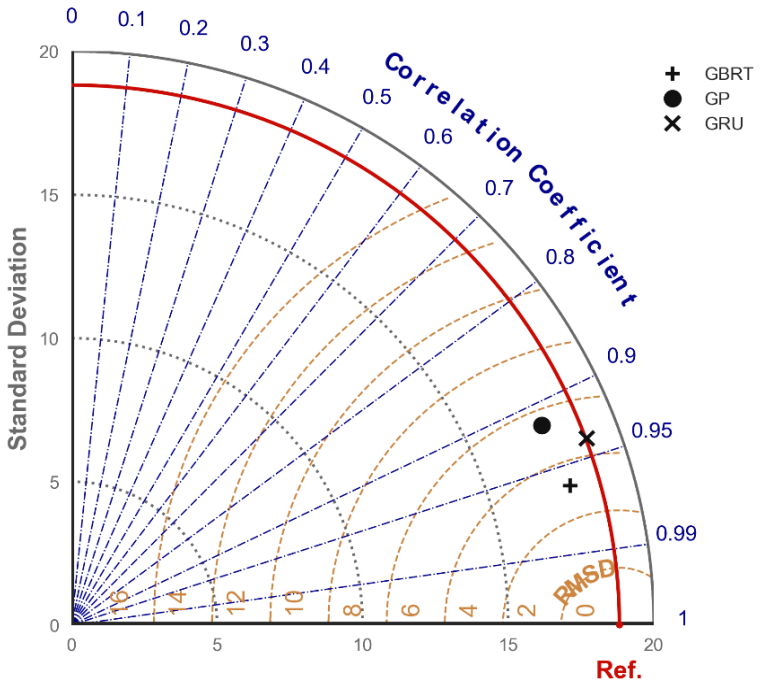

Figure 3-11: Taylor diagram comparing performance of the developed ML models.

3.5.3 Comparison with Previous Studies

A prime goal in ML is to create models that can accurately predict the output for new unseen data never presented to the model, *i.e.*, achieving models that can generalize (Chollet, 2018). ML models generalize a phenomenon through learning the underlying principles within the training data. Hence, they are capable of generalizing when predicting sensible outputs from inputs different than those of the training dataset (Marsland, 2015). Testing the model on a high number of unseen data samples is the rational way to determine whether the model is generalizing or not, thus the importance of having large datasets (Marsland, 2015). The models proposed in the present chapter have demonstrated better generalization capability than those informer studies. A major reason for this superior performance is that the test dataset used in this study has more data samples than the entire datasets used in developing previous models, including Khademi et al. (2016), Z H Duan

et al. (2013), Deshpande et al. (2014), Topçu and Saridemir (2008), Deng et al. (2018), and Naderpour et al. (2018), (see **Table 3-14**). It is important to mention that Deng et al. (2018) was not included in **Table 3-14** because they neither report the coefficient of determination nor the root mean squared error. However, they reported the relative percentage error, which corresponded to 6.63, 4.35, and 3.65 for the black propagation neural network, support vector machine, and convolutional neural network, respectively.

Table 3-14: Comparison of statistical measurements with previous studies

Machine Learning Technique	R^2	*RMSE*	Samples	References
Multiple linear regression	0.609	9.975	257	Khademi *et al.*, 2016
Artificial neural networks	0.919	4.446		
Adaptive neuro-fuzzy inference system	0.908	5.045		
Artificial neural networks	0.995	3.6804	168	Z H Duan *et al.*, 2013
Artificial neural networks	0.903	-	257	Deshpande *et al.*, 2014
Model tree	0.757	-		
Non-linear regression model	0.740	-		
Artificial neural networks	0.998	2.395	210	Topçu and Saridemir, 2008
Fuzzy logic	0.996	3.866		
Artificial neural networks	0.688	-	139	Naderpour *et al.*, 2018
Artificial neural networks	0.971	-	1178	Dantas *et al.*, 2013
Multivariate adaptive regression splines	-	8.750	650	Gholampour *et al.*, 2018
M5 model tree	-	8.250		
Least support vector regression	-	7.550		
Gradient Boosting[a]	**0.919**	**5.076**	**1134**	**-**
Deep Learning[a]	**0.868**	**6.502**		

[a] model of the present thesis

Table 3-14 shows the coefficient of determination and the root mean squared error of models in previous studies that predicted the compressive strength of RAC. It can be observed that models in the present thesis achieved better accuracy than that of Gholampour *et al.* (2018) and Deshpande *et al.* (2014) who used relatively large data samples. As expected, the studies that reported a shorter database reached higher accuracy. For instance, Duan *et al.* (2013) and Khademi *et al.* (2016) used 168 and 257 samples, respectively. The reported accuracy was 0.995 for Duan *et al.* (2013) and 0.919 for Khademi *et al.* (2016), both studies using ANNs. This indicates that although higher number of samples might result in a better generalized model, the accuracy can decrease, and thus accuracy metrics alone might not be enough to assess predictive models. Also, several models which used smaller data sets than that in the present thesis, including Khademi *et al.* (2016), Duan *et al.* (2013), Deshpande *et al.* (2014), Topçu and M.

Saridemir (2008), Deng *et al.* (2018), and Naderpour *et al.* (2018), had compromised generalization capability. Furthermore, in the case of Gholampour *et al.* (2018), the authors decided to split the available data and create two different models to predict the compressive strength of those samples corresponding to cylindrical specimens and those corresponding to cube specimens. Conversely, the present study considered the specimen type as an input feature, resulting in higher accuracy. Generally, the present study along with Dantas *et al.* (2013) used the highest number of data. However, Dantas *et al.* (2013) reported a coefficient of determination higher for the testing set than that for the training set, 0.971 and 0.928, respectively. This is a sign that their model was not sufficiently trained, as suggested by Gulli and Pal (2017).

3.5.4 RAC Mixture Proportioning and Optimization

A PSO was coupled with the GBRT model to optimize the mixture design and predict the compressive strength of RAC, such that the most economic mixture proportion is obtained for a given compressive strength class. The optimization was performed considering the unit costs of materials presented in **Table 3-7**. Not only does the optimization process reduce the higher unit cost ingredients, but it also reduces cement in the mixture, providing both economic benefit and sustainable mixture designs with less CO_2 emission. High upper limit of recycled aggregate was considered in the optimization to ensure maximum replacement of recycled aggregates as presented in **Table 3-8**. Although using higher portions of recycled aggregate may contradict with compressive strength requirements, the optimization was carried out to maintain highest possible recycle aggregate content along with the desired compressive strength class.

Table 3-9 presents the optimized mixture designs of RAC for different compressive strength classes as obtained by the PSO model. The mixture proportions were then used to predict the compressive strength using the GBRT model. Silica fume was not considered in the optimization process, and thus was set to zero when predicting the compressive strength with the GBRT model. Ultimately, considerable reduction of cost in all cases, especially for the lower compressive strength range, was achieved as outlined in **Table 3-10**. For instance, there was 25% reduction in the cost of the RAC mixture without affecting its compressive strength when the target compressive strength was 35 MPa. The

optimization process demonstrated the outstanding capability of the PSO-GBRT model in capturing complex relationships within the data to select the best mixture proportions, while maintaining a similar water-to-cement ratio to that of the base mixture. This can be observed for instance when considering the 25 and 30 MPa compressive strength classes in which high water-to-cement ratio was proposed with high RCA content having high water absorption capacity, as observed in experimental studies (Poon *et al.*, 2004).

3.6 Conclusions

The present study explores deploying state-of-the-art machine learning models to predict the compressive strength of RAC. For this purpose, one of the largest existing experimental datasets including 1134 mixture design examples and featuring 10 attributes was built from studies in the open literature. Three advanced machine learning models, including Gaussian processes (GP), deep learning (DL), and gradient boosting regression trees (GBRT), were tuned, trained, and tested using the dataset. To guarantee that the developed models were able to generalize the compressive strength of RAC, *K*-fold cross-validation was used during the tuning process. The results show that the three models successfully captured the underlying principles contributing to the compressive strength of RAC. Furthermore, the diverse nature of the algorithms used herein proves the robustness of ML algorithms for data analysis despite the complexity within the dataset. The comparison of the models' performance revealed that the GBRT and DL (recurrent neural network) models had a superior performance compared to GP model in terms of different performance indicators. Accordingly, the obtained coefficient of determination of the testing set for GBRT, DL, and GP was 0.919, 0.868, and 0.844, respectively. Furthermore, GBRT model was coupled with a PSO to create a hybrid model for optimizing the mixture design of RAC with various compressive strength classes. Accordingly, the GBRT-PSO hybrid model successfully proposed economic mixture designs that fulfill the compressive strength requirement, reduce cost, and mitigate the environmental footprint of concrete production. To further the high potential of the developed ML models, it is proposed to integrate supplementary cementitious materials, such as fly ash and blast furnace slag in the dataset, and to extent the models to also capture durability requirements of RAC in future work.

3.7 Chapter References

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Chapter 4

4 Machine Learning Prediction of Carbonation Depth in Recycled Aggregate Concrete Incorporating SCMs

The rapid growth of the concrete industry has caused several environmental issues, such as the depletion of natural aggregates, overload of landfills, and CO_2 emission released to the atmosphere (Duan *et al.*, 2013; Naderpour *et al.*, 2018; Pedro *et al.*, 2015). One latent solution to decreasing the environmental footprint of concrete production is the reuse of construction and demolition waste (CDW) as recycled aggregate. The undisputed environmental advantages of using recycled aggregate concrete (RAC) has attracted the attention of researches over the last four decades (R. V. Silva *et al.*, 2015). However, most studies have stablished that the use of recycled aggregates (RAs) diminishes some properties of concrete. The disadvantages of using RAs as partial replacement for natural aggregates (NAs) have hampered its wider use in structural concrete (S.C. Kou and Poon, 2012; Thomas *et al.*, 2013). Whilst, most studies have focused on exploring the mechanical properties of RAC, there is growing awareness that durability-related properties of concrete are more affected by the inclusion of RAs (Amorim *et al.*, 2012; S.C. Kou and Poon, 2012).

One of the main goals of the circular economy is to extend the service life of structures, which can be achieved by fully understanding the effects of different factors influencing the durability of concrete (Sáez del Bosque *et al.*, 2020). The three-vector approach proposed by Santos *et al.* (2019) to develop more concrete technologies included: increase the durability of concrete, lower energy consumption in its production and placement processes, and recycling materials. These vectors highlight the need for a concerted sustainable development strategy of the concrete industry. Indeed, concretes with poor durability require costly maintenance (Torgal *et al.*, 2012) Thus, sustainable development and reduction of maintenance costs go hand in hand and are enhanced through improving the concrete durability.

Several deterioration mechanisms are involved in compromising the durability of concrete, such as physical and chemical attack and exposure to hostile environments (ACI Committee, 2016; R. V. Silva *et al.*, 2015). Ingress of chloride ions, carbonation, freezing-

thawing cycles, sulfate attack and alkali-aggregate reaction are chief among the concrete durability-related issues in northern environments (Abbas *et al.*, 2009a). Although chloride ions penetration is known to be more aggressive, most structures are more likely to incur carbonation attack than exposure to chloride ions penetration (Sáez del Bosque *et al.*, 2020; R. V. Silva *et al.*, 2015). However, damage originates not only from external environmental factors, but also can be instigated by concrete ingredients and inner microstructure (R. V. Silva *et al.*, 2015).

A critical look at studies on the durability performance of RAC indicates that they have several discrepancies in their conclusions, with limited analysis and comparison of the available information (Thomas *et al.*, 2013). Whilst some studies claim that the inclusion of RAs diminishes the concrete durability (Arredondo-Rea et al., 2012; Muduli and Mukharjee, 2020; Otsuki *et al.*, 2003), others posit that the use of high-quality RA did not contribute to decreasing durability properties (Levy and Helène, 2007; Matias *et al.*, 2014). The factors contributing to these contradictory conclusions include the different exposure conditions of specimens tested by different researchers, the different mixture ingredients and their proportioning, the composition and inherent variability of RAs, and several specific processes involved in the production of RAC, such as the crushing method or the mixture design method (Torgal *et al.*, 2012). Moreover, the available information on the effect of different types of binders on the properties of RAC has several discrepancies. For instance, Malhotra *et al.* (2000) reported that the inclusion of fly ash had negligible effect on the carbonation resistance of concrete, while Khunthongkeaw et al. (2006) reported that the carbonation coefficient increased proportionally with the dosage of fly ash.

Therefore, to elucidate the effects of RA and different types of SCMs, the present study proposes a machine learning (ML) model to predict carbonation depth based on 713 experimental records retrieved from the literature. Both accelerated carbonation tests as well as outdoor exposure carbonation tests were considered in the gathered data. A major advantage of ML methods is that it can capture the underlying mechanisms, despite the lack of clarity of specific information, and can generalize the data structure (Kumar *et al.*, 2019). Data driven ML techniques have proven to be successful in predicting RAC mechanical properties, such as the modulus of elasticity and compressive strength, as well

as determining the quality characteristics of concrete (Dantas *et al.*, 2013; Gholampour *et al.*, 2018; Song *et al.*, 2020). In this chapter the effects of four types of binders, including fly ash, metakaolin, blast furnace slag, and silica fume on the carbonation resistance of RAC via a gradient boosting regression tree (GBRT) model are examined.

4.1 Carbonation

Carbonation is a physical-chemical process prompted by the reaction of hydrated cementitious composites with carbon dioxide (Amorim *et al.*, 2012) This process starts at the surface of concrete members and extends through its core at a rate controlled by the concrete porosity, alkaline reserve of the cementitious paste, relative humidity, concentration of CO_2, and other exposure conditions (Marinković *et al.*, 2017). The carbon dioxide (CO_2) from the atmosphere or dissolved in water reacts with calcium hydroxide in the concrete matrix, forming calcite ($CaCO_3$) (Devi and Khan, 2020), see **Figure 4-1**. As calcite is generated, the alkalinity of the concrete decreases, possibly reaching pH lower than 9. In reinforced concrete (RC) structures, the high alkalinity of concrete passivates the steel reinforcement, while the loss of alkalinity can result in reinforcement de-passivation and risk of corrosion (Carevic *et al.*, 2019). Reinforcement corrosion is the most common and costly degradation mechanism of concrete, resulting in multi-billion-dollar losses worldwide and a colossal backlog of damaged structures (Monteiro et al., 2012)

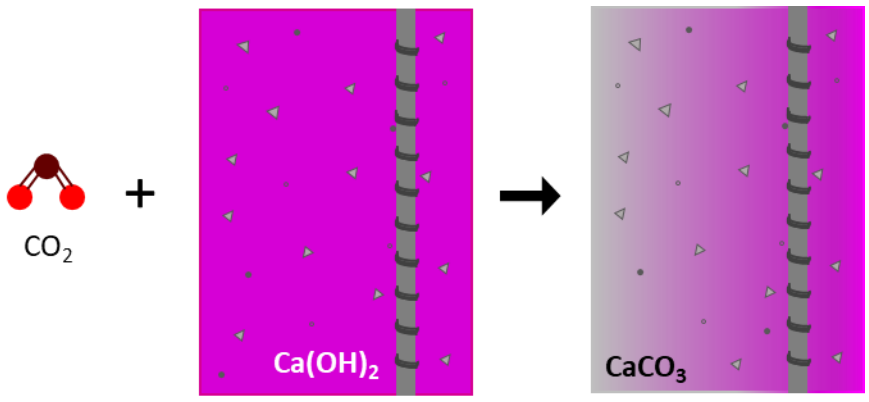

Figure 4-1: Carbonation process.

The two main causes of corrosion in RC structures are chloride penetration and carbonation (ACI Committee, 2016). Although chloride penetration is known to be more aggressive, carbonation is more common (R. V. Silva *et al.*, 2015). Hence, several studies have aimed at developing analytical models for determining the carbonation depth of concrete. Most of these models are created after Fick's first law, in which the base model considers the carbonation depth to be a function of the squared root of time:

$$x = K\sqrt{t} \quad \textbf{(4-1)}$$

where, x is the carbonation depth, t is the exposure time and K is the carbonation coefficient, which in turn depends on the concentration of CO_2 and the diffusion characteristics of the concrete (Monteiro *et al.*, 2012). Various researchers have proposed several variants of this model considering the most determinant factors on the carbonation depth. In this thesis, three analytical models were selected to determine the carbonation depth of the experimental conditions the retrieved database. Their calculations were compared with the predictions of the proposed machine learning model.

Czarnecki and Woyciechowski (2012) proposed a model that assumes limited carbonation depth based on the premise that the pores of concrete become filled with carbonation products once the deterioration mechanism starts. This model considered one qualitative and two quantitative characteristics, including, the type of binder, water-to-binder ratio, and time of water curing. The model was tested on different concrete types, covering three types of binder, three ages of curing, and three water-to-binder ratios. Both the water-to-binder ratio and curing time had a high effect on the carbonation depth, with a coefficient of determination within the range of 0.85-0.94. The equation to determine the carbonation depth of 2-days-curing concrete using the exposure time and the water-to-cement ratio for Portland cement is expressed as follows:

$$x = -0.56213 - \frac{8.792}{\sqrt{t}} + 17.8372\left({}^{w}/_{b}\right) \quad \textbf{(4-2)}$$

In another study, Woyciechowski et al. (2019) described the process of carbonation of concrete containing fly ash. Experimental tests were carried out to determine the

compressive strength, tensile strength, and carbonation depth of 10 different concrete mixture compositions. The results obtained through the accelerated carbonation test were then used to formulate a hyperbolic model with the water-to-cement ratio $\left(w/_b\right)$ and fly ash-to-cement mass ratio $\left(fa/_c\right)$ as the independent variables. The authors recommended using their proposed formulation as a starting point to determine safe thickness of concrete covers. They also suggested using safety factors to account for other characteristics of concrete, especially those related to the curing process. The equations proposed by Woyciechowski et al. (2019) for 56 and 90 days of exposure are, respectively:

$$x = 46.57 - 103.85\left(w/_b\right) - 150.88\left(fa/_c\right) + 90.05\left(w/_b\right)^2 + 159.16\left(w/_b\right)\left(fa/_c\right) + 107.87\left(fa/_c\right)^2 \quad \textbf{(4-3)}$$

$$x = -10.46 + 102.55\left(w/_b\right) - 76.24\left(fa/_c\right) - 92.35\left(w/_b\right)^2 + 62.31\left(w/_b\right)\left(fa/_c\right) + 58.29\left(fa/_c\right)^2 \quad \textbf{(4-4)}$$

A RILEM report (Sarja and Vesikari, 1996) was dedicated to the durability of concrete structures and examined the available durability models to incorporate the degradation of materials into the design of structures. This report highlighted the importance of determining the durability parameters, e.g., depth of deterioration of concrete and detailing of reinforcing rebar, to satisfy a given design service life, considering the environmental exposure on the structure. This report presented several models to evaluate the carbonation depth of concrete. Only the model expression in **Eq. 4-5** was considered herein:

$$x = (C_{env}C_{air}\ a\ {f_c}^b)\sqrt{t} \quad \textbf{(4-5)}$$

Here C_{env} and C_{air} are the environmental coefficient and the air content coefficient, respectively, a and b are parameters that depend on the binding agent, f_c is the cubic compressive strength, and t is the exposure time. For portland cement, a and b are equal to 1800 and -1.7, respectively. The environmental coefficient is equal to 1 for structures sheltered from rain and 0.5 for structures exposed to rain. Similarly, the air content coefficient is 1 for non-air-entrained and 0.7 for air-entrained concrete. The values for the coefficients a and b are provided in **Table 4-1**.

Table 4-1: Parameters a and b used to determine carbonation depth

Binder type	*a*	*b*
Portland cement	1800	-1.7
Portland cement and 28% fly ash	360	-1.2
Portland cement and 9% silica fume	400	-1.2
Portland cement and 70% blast furnace slag	360	-1.2

4.2 Gradient Boosting

Gradient boosting regression tree (GBRT) algorithm is a sequential ensemble of decision trees that uses a boosting approach, where the prime goal is to find a function, F_M, that minimizes the loss function $L(y, F(\boldsymbol{x}))$ (Zhan *et al.*, 2020). Gradient boosting considers additive decision trees, see **Figure 4-2**, commonly referred as base learners or weak learners, that approximate a prediction of the form:

$$F_M(x) = \sum_{m=0}^{M} \beta_m \, h(\boldsymbol{x}; a_m) \qquad \textbf{(4-6)}$$

where $h(\boldsymbol{x}; a_m)$ refers to the decision tree with its respective parameter a_m, and β_m represents the expansion or weighting coefficients (J.H. Friedman, 2002). The weighting coefficients and the base learners are fitted to the training data x in a greedy manner as follows:

$$F_m(\boldsymbol{x}) = F_{m-1}(\boldsymbol{x}) + \beta_m \, h(\boldsymbol{x}; a_m) \qquad \textbf{(4-7)}$$

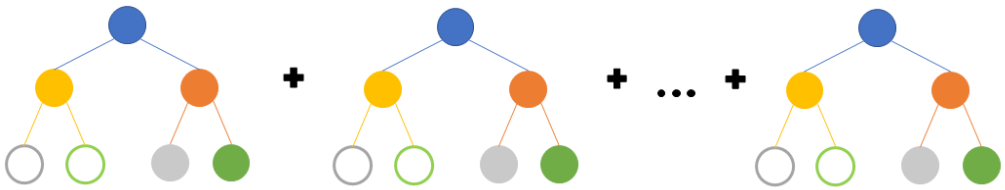

Figure 4-2: Addition of regression trees for Gradient Boosting.

The GBRT is optimized by the steepest descent method, such that the next decision tree is built by fitting the input variable $\boldsymbol{x}$ and the negative gradient of the last model's loss

function $z_m\ (x_i)$, mentioned below (Zhan *et al.*, 2020). The weighting coefficients, β_m, are obtained through **Eq. 4-9.**

$$z_m(x_i) = -\frac{\partial L(y,F_{m-1}(x_i))}{\partial F_{m-1}(x_i)} \quad \textbf{(4-8)}$$

$$\beta_m = argmin\ \sum_{i=1}^{N} L(\ y, F_{m-1}(x_i) - \beta\ h(x_i; a_m)) \quad \textbf{(4-9)}$$

The fitted regression tree and the gradient descent step size are then used to update the model $F_m\ (\boldsymbol{x})$ (Zhan *et al.*, 2020). Thus, the GBRT adds basic learners to minimize any differentiable loss function, $L(y, F(\boldsymbol{x}))$, using a given dataset $\{(x_1, y_1), (x_2, y_2), \dots, (x_N, y_N)\}$ (J. Friedman, 2001; J.H. Friedman, 2002).

4.3 Data Collection

Several types of binders were considered in the collected experimental data-records to study their influence on the carbonation of RAC, including blast furnace slag, fly ash, metakaolin, silica fume and Portland cement. From the collected data samples, 4%, 30%, 2%, and 1% reported using blast furnace slag, fly ash, metakaolin, and silica fume, respectively.

According to Alexandridou *et al.* (2018), the significantly different conditions to carry out the accelerated carbonation test do not allow for objective comparison of the available data. Thus, the carbon concentration at which the experiments were performed as well as the exposure time were also considered as attributes of the collected data.

It is believed that the intrinsic porosity of aggregates is closely related to the carbonation resistance of RAC (Amorim *et al.*, 2012). Hence, the water absorption and density of the aggregate were contemplated as an input features of the retrieved data-records. However, to account for the aggregate content along with its physical properties, the particle density and water absorption of both natural coarse aggregates and recycled coarse aggregate were calculated via the following equations:

$$\Upsilon_{CA} = \Upsilon_{NCA}(1 - r) + \Upsilon_{RCA}(r) \quad \textbf{(4-10)}$$

$$WA_{NCA} = \frac{wa_{NCA}(NA)}{\Upsilon_{NCA}} \quad \textbf{(4-11)}$$

$$WA_{RCA} = \frac{wa_{RCA}(RCA)}{\Upsilon_{RCA}} \quad \textbf{(4-12)}$$

Here Υ_{CA} is the density of the coarse aggregate considering the particle density of both the natural coarse aggregate, Υ_{NCA} , and the recycled coarse aggregate, Υ_{RCA}, as well as their respective volume fraction r (%). WA_{NCA} and WA_{RCA} are the water absorption times the mixed volume of natural coarse aggregate and recycled coarse aggregate, respectively. The volume of the coarse aggregate used was calculated by the ratio between either the natural or recycled coarse aggregate content and its respective particle density.

Some authors have claimed that there is a relationship between the compressive strength and durability properties of concrete (Santos *et al.*, 2019; R. V. Silva *et al.*, 2015). Therefore, the compressive strength was also considered as an input feature for the ML model presented herein. Within the data-records, some authors reported the cylindrical compressive strength, whilst some others reported the cube compressive strength. Thus, following the recommendations given by Pacheco *et al.* (2019) for RAC, the cylindrical compressive strength was converted to cube compressive strength diving it by 0.77:

$$f'c_{cube} = \frac{f'c_{cylinder}}{0.77} \quad \textbf{(4-13)}$$

Conclusively, the collected data used in this study consisted of 713 examples with 17 input features and one output retrieved from 20 peer-reviewed publications (Abbas *et al.*, 2009b; Alexandridou *et al.*, 2018; Arredondo-Rea *et al.*, 2012; Bravo *et al.*, 2015; Buyle-Bodin and Hadjieva-Zaharieva, 2002; Carevic *et al.*, 2019; de Brito and Evangelista, 2012; Devi and Khan, 2020; Jianzhuang *et al.*, 2012; S. Kou and Poon, 2013; S.C. Kou and Poon, 2012; Limbachiya *et al.*, 2012; Matias *et al.*, 2014; Muduli and Mukharjee, 2020; Otsuki *et al.*, 2003; Pedro *et al.*, 2015, 2017; Sáez del Bosque *et al.*, 2020; Zhang and Zong, 2014; Zhu *et al.*, 2013), see **Table 4-2**. Statistical characteristics of the data set are given in **Table 4-3**. Analysis to identify whether there existed any association between the attributes listed in **Table 4-3** was carried out using the Pearson correlation coefficient, see **Figure 4-3**. This

analysis unveiled high correlation between the compressive strength and water-to-binder ratio of the concrete and its carbonation depth. Contrarily, the aggregate, silica fume, and fly ash contents had insignificant association with the carbonation depth.

Table 4-2: Sources of experimental data retrieved in this thesis to build experimental database

References	No. of Samples
Bravo *et al.*, 2015	84
Pedro *et al.*, 2015	72
de Brito and L. Evangelista, 2012	16
F. Buyle-Bodin and R. Hadjieva-Zaharieva, 2002	6
S. C. Kou and C. S. Poon, 2013	40
Matias *et al.*, 2014	11
Otsuki *et al.*, 2013	8
Abbas *et al.*, 2009b	98
Arredondo-Rea *et al.*, 2012	32
Jianzhuang *et al.*, 2012	40
Limbachiya *et al.*, 2012	144
Muduli and Mukharjee, 2020	22
Devi and Khan, 2020	8
Sáez del Bosque *et al.*, 2020	12
Carevic *et al.*, 2019	8
Alexandridou *et al.*, 2018	16
Zhu *et al.*, 2013	6
S. C. Kou and Poon, 2012	60
Zhang and Zong, 2014	18
Pedro *et al.*, 2017	12

4.3.1 Data Preprocessing and Hyperparameter Tuning

Feature normalization is known to improve computational efficiency of machine learning models (Marsland, 2015), see **Figure 4-4**. Accordingly, the statistical standardization method was used in this study to normalize the collected data-records prior to GBRT modeling. Statistical standardization transforms the data computing the deviation from the mean, such that the standard deviation is set equal to 1 and the mean equal to 0 (Shanker *et al.*, 1996). The data was randomly partitioned into training and testing sets: 70% of the data was used for training (499 samples) and the remaining was used for testing (214 samples).

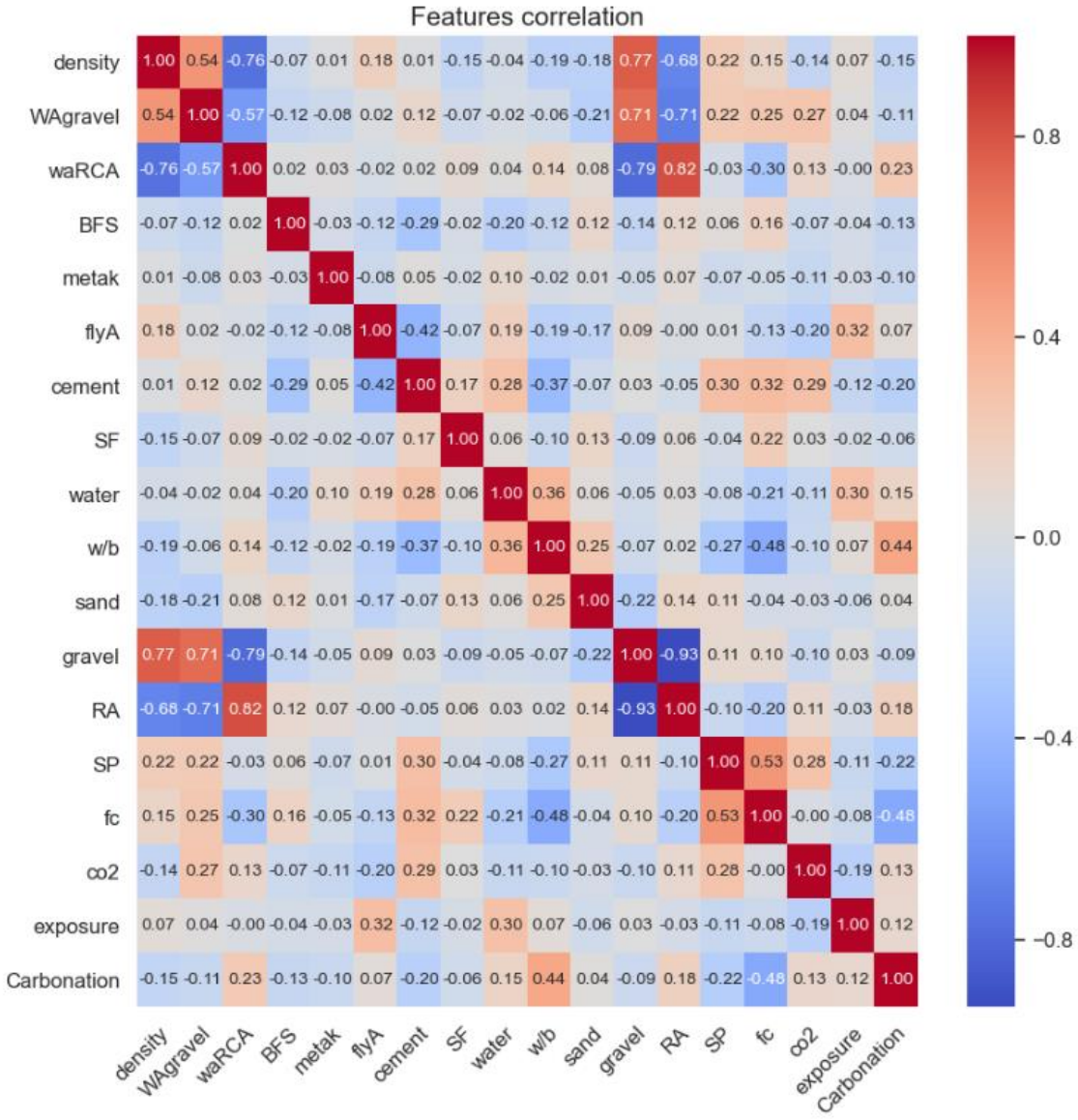

Figure 4-3: Pearson correlation coefficient for the dataset attributes.

Table 4-3: Statistical parameters of input features

Feature	Units	Min.	Max.	Mean	Standard deviation
Weighted density	kg/m^3	1928.00	2860.00	2461.78	143.40
Water absorption, gravel	% * m^3	0.00	2.55	0.18	0.23
Water absorption, RCA	% * m^3	0.00	4.62	1.34	1.06
Blast furnace slag	kg/m^3	0.00	125.00	4.77	23.62
Metakaolin	kg/m^3	0.00	84.00	1.18	8.54
Fly ash	kg/m^3	0.00	225.50	34.32	57.70
Cement	kg/m^3	133.00	558.00	331.71	74.04
Silica fume	kg/m^3	0.00	62.00	0.67	5.70
Water	kg/m^3	66.50	280.00	184.19	29.64
Water-to-binder ratio	-	0.25	1.02	0.51	0.11
Sand content	kg/m^3	357.66	998.00	653.43	175.34
Gravel content	kg/m^3	0.00	1311.00	473.98	442.49
Recycled aggregate content	kg/m^3	0.00	1280.00	561.18	415.68
Superplasticizer	kg/m^3	0.00	7.31	0.89	1.81
Compressive strength	MPa	18.01	131.36	42.37	13.23
CO_2 content	%	0.04	50.00	5.30	6.34
Exposure time	Days	7.00	3650.00	171.07	528.05
Carbonation depth	mm	0.10	50.06	10.29	8.32

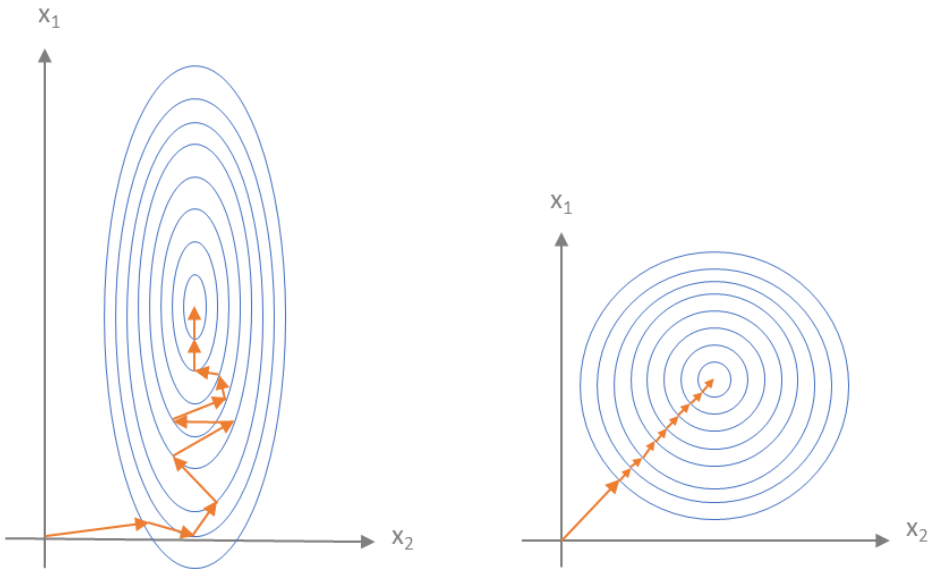

Figure 4-4: Feature normalization.

The optimum model hyperparameters for the GBRT model were selected through a tuning process assisted by a 5-fold cross-validation (CV) technique using the `Scikit-learn` package in Python (Varoquaux *et al.*, 2015). Typically, ML models are divided into training, validation and testing sets (Marsland, 2015). The model learns from the training

set, then the validation set is used to estimate the prediction error, and the testing set is used to assess the generalization capability of the model (Hastie *et al.*, 2008). However, for cases with insufficient data, partitioning the data into 3 sets might leave the training set without enough samples to learn appropriately. In such a case, K-fold CV is an excellent alternative technique (Hastie *et al.*, 2008). In K-fold CV, the data is split into K equal-sized subsets such that K-1 subsets are used for training and the remainder of these is kept for validation.

Whilst the partitioning of the data into training and testing sets was done randomly to ensure that the training set included representative samples from the original data set, the tuning process was executed over 5 different random seeds. Accordingly, a randomized search procedure was used to determine the optimal hyperparameters for the GBRT model. Random search along with grid search algorithms are among the most widely used hyperparameter automatic search techniques (J. Bergstra *et al.*, 2013). The former chooses the hyperparameter trials randomly and has proven to be more efficient than grid search since it explores all possible hyperparameter values (James Bergstra and Bengio, 2012).

4.3.2 GBRT Model Development

GBRT modeling and tuning was performed using Scikit-learn package in Python (Varoquaux *et al.*, 2015). The most significant hyperparameters affecting the predictive performance of a GBRT model are the number of trees, known as number of estimators in Scikit-learn package, the learning rate, and the max depth of the tree (Zhan *et al.*, 2020). Whilst larger number of trees increases the prediction accuracy of the model, excessive trees could result in an over-fitted model with lack of predictive capacity for new unseen data. The max depth indicates the complexity of each tree and the learning rate controls the contribution of each tree to the predictions. Similar to the number of trees, immoderate values of such hyperparameters reduce the prediction accuracy of the GBRT model (Zhan *et al.*, 2020). **Table 4-4** presents the tuned values for the GBRT model used herein.

The performance of the GBRT model was then evaluated using three different statistical metrics, including the coefficient of determination (R^2), the mean absolute error (MAE), and the root mean squared error ($RMSE$) as expressed below in equations 15, 16 and 17, respectively (Cai *et al.*, 2020; Renaud and Victoria-Feser, 2010):

$$R^2 = 1 - \frac{\sum(y-y')^2}{\sum(y-\bar{y})^2} \quad \textbf{(4-15)}$$

$$MAE = \frac{1}{n}\sum|y - y'| \quad \textbf{(4-16)}$$

$$RMES = \sqrt{\frac{1}{n}\sum(y - y')^2} \quad \textbf{(4-17)}$$

Table 4-4: Optimized hyperparameters for GBRT model

Hyperparameter	Value
Number of estimators	3575
Learning rate	0.1
Min samples split	5
Min samples leaf	1
Max depth	4
Max features	8
Loss function	Huber
Alpha	0.94
Subsample	1
Criteria function	Friedman MSE

4.4 Results and Discussion

As outlined previously, the GBRT model was trained attempting to predict the carbonation depth of 214 unseen experiments. This section aims at discussing the results obtained from such implementation, as well as to analyze and compare with former analytical models to determine the carbonation depth of concrete.

4.4.1 Prediction Performance of GBRT Model

The GBRT model was trained on 499 data-records and tested on the remaining 214 samples. To assess the robustness of the model, it was performed over 5 different random seed numbers. Random seeds are used to obtain reproducible results in ML methods by initializing the random number generator (Lee and Kim, 2005; M.L. Silva *et al.*, 2020). In this study, five different random seeds were used: 1009, 3090, 999, 5341, and 1200. The quantitative measurements for the five different seeds are presented in **Table 4-5**. For the testing set, the GBRT model predicted the carbonation depth with average $RMSE$, MAE, and R^2 values of 1.5139, 0.948, and 0.9707, respectively. For the training set, the results were 0.0822, 0.0249, 0.999 for $RMSE$, MAE, and R^2, respectively. The distribution of the

residuals for both the training set and testing set are depicted in **Figure 4-5**. This figure demonstrates the superior accuracy achieved by the GBRT model. Accordingly, **Figure 4-6** shows the actual versus predicted carbonation depth for the testing set of random seed equal to 1200. This study demonstrates that the GBRT model can be a powerful tool for determining the carbonation resistance of concrete incorporating RCA. For prediction of carbonation depth of RAC, no comparable model was found.

4.4.2 Feature Importance

GBRT demonstrated to be a powerful framework to capture the underlying mechanisms that determine the carbonation depth of RAC made with several types of binder. Nonetheless, the GBRT algorithm is rather considered a black-box model due to the lack of comprehensibility of its prediction process (Strobl *et al.*, 2008). and the absence of an explicit equation that can be transparently used for prediction. Whilst regression trees can be interpreted by analyzing their structure, GBRT models are typically comprised of thousands of regression trees. Thus, the visualization of all the trees can be a daunting task (Auret and Aldrich, 2011).

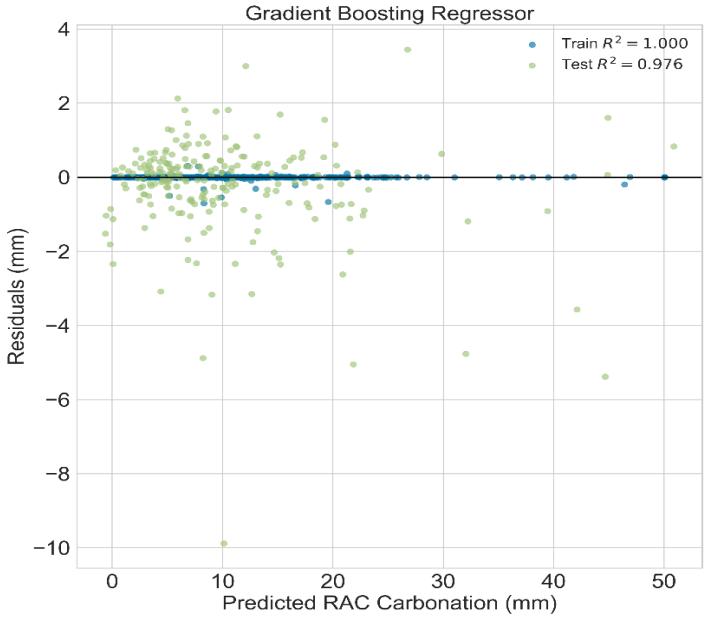

Figure 4-5: Residuals plot for GRBT model, testing dataset.

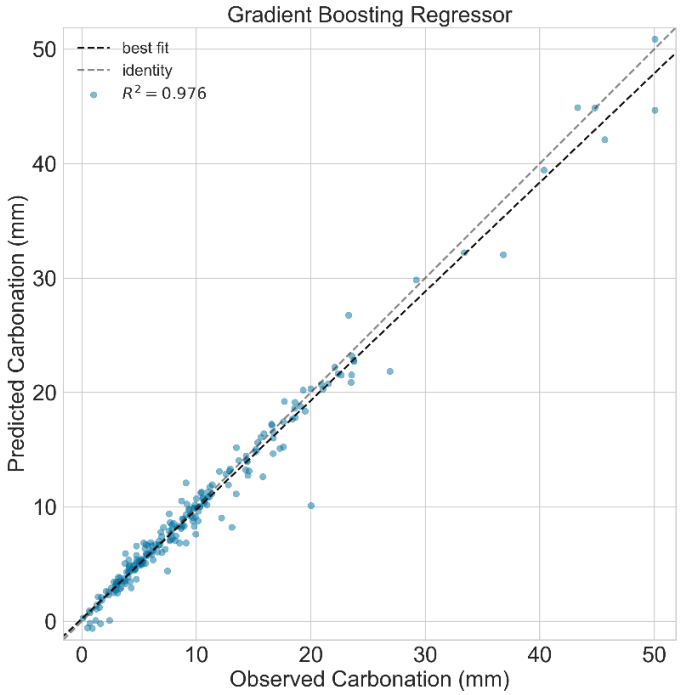

Figure 4-6: Residuals plot for GBRT model, testing dataset.

Table 4-5: Measured performance of GBRT

Random Seed and Global Performance	Set	*RMSE*	*MAE*	R^2
RS[a] = 1009	Test	1.4128	0.9122	0.9728
	Train	0.0647	0.0149	0.9999
RS[a] = 3090	Test	1.5114	0.9190	0.9654
	Train	0.0607	0.0126	0.9999
RS[a] = 999	Test	1.7343	1.0216	0.9662
	Train	0.1196	0.0481	0.9998
RS[a] = 5341	Test	1.5289	0.8395	0.9732
	Train	0.1022	0.0331	0.9998
RS[a] = 1200	Test	1.3819	0.8314	0.9758
	Train	0.0638	0.0157	0.9999
Average	**Test**	**1.5139**	**0.9048**	**0.9707**
	Train	**0.0822**	**0.0249**	**0.9999**
Standard Dev	**Test**	**0.1382**	**0.0767**	**0.0046**
	Train	**0.0269**	**0.0153**	**0.0001**

[a] random seed [b] root mean squared error [c] mean absolute error

However, several procedures have been widely used to interpret predictions from tree ensemble methods (Huynh-Thu *et al.*, 2012) In the present study, the Scikit-learn package was implemented to determine the feature importance of the input attributes used herein, as shown in **Figure 4-7**. In the `Scikit-learn` library, the mean decrease impurity index is used to determine the relative importance of the input features. This measurement considers the relative depth of the feature along with its contributed splits (Louppe, 2014). **Figure 4-7** depicts the index of the input feature on the ordinate axis, thus, the three corresponding attributes with the highest impact in descending order are: Exposure time (days); Compressive strength (MPa); and Water-to-binder ratio.

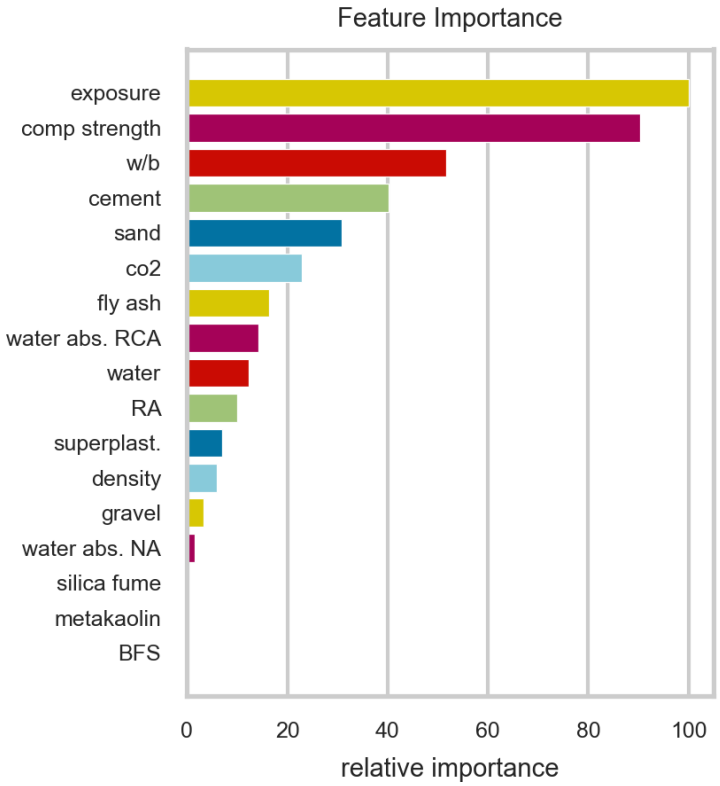

Figure 4-7: Feature importance.

In the retrieved experimental data from the open literature, there was not sufficient studies on the carbonation resistance of RAC with the inclusion of supplementary cementitious materials. Thus, the GBRT model was not able to appropriately capture the effect of these types of composites on the predicted carbonation depth for the experimental samples studied herein. Yet, this did not avert the algorithm to learn the underlying mechanisms

involved in the carbonation process of RAC, regardless the type of binder. This model limitation could be mitigated when pertinent experimental data becomes available in the open literature.

4.4.3 Comparison to Analytical Models to Determine Carbonation Depth

The three different theoretical models mentioned earlier in section 2 were assessed and their calculation was compared with predictions of the ML model proposed herein in the determination of the carbonation depth of concrete specimens. The formulations proposed by Czarnecki and Woyciechowski (2012), Woyciechowski *et al.* (2019), and the expressed in the RILEM report edited by Sarja and Vesikari (1996) were used to determine the carbonation depth of experimental records from the experimental database created in this study. The selection of samples used to determine the carbonation depth was done in concordance with the experiments conducted to reach such analytical models. For instance, Woyciechowski *et al.* (2019) described 3 models of carbonation depth for concrete with a water-to-cement ratio within the range of 0.35 to 0.55, fly ash-to-cement mass ratio values from 0.2 to 0.5, and 56, 70, and 90 days of exposure in a carbonation chamber with CO_2 concentration of 4%. Thus, this analytical model was performed over the sixteen data-records that met those characteristics. Only the two models described in **Eq. 4-3** and **Eq. 4-4** were used since there were no experimental data sets that met the above-mentioned requirements with 70 days of exposure.

Figure 4-8 displays the predictions obtained using these equations, *y_pred*, and the values form the experimental data, *y*. Accordingly, the model proposed by Czarnecki and Woyciechowski (2012) was developed after testing concrete specimens exposed to outdoor environmental conditions with 2 days of water-curing before the exposure. For this formulation, 48 data samples were found to meet these requirements. **Figure 4-9** plots the predictions, *y_pred*, and the experimental carbonation depth of 48 different samples, *y*. The formulation found in the RILEM report is dependent on the cube compressive strength of concrete, the environmental conditions, air entrainment, and the binder type. Therefore, only data-records that included the cube compressive strength of samples made with portland cement were used. The environmental coefficient and the air content coefficient

were considered both equal to 1. Also, the original study where this formulation was first published, Häkkinen (1993), determined the carbonation depth of concrete exposed to a concentration of carbon dioxide of 3%. Hence, 72 samples that met the former requirements were chosen. **Figure 4-10** depicts the carbonation depth determined with this formulation, *y_pred*, and the experimental results, *y*.

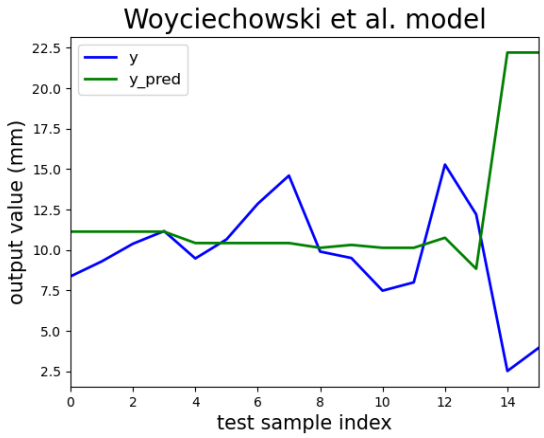

Figure 4-8: Actual and predicted values using the formulation proposed by Woyciechowski *et al.* (2019).

All the aforementioned analytical models for calculating the carbonation depth of concrete were based on Fick's first law. One of the most important limitations of using this law is the consideration that carbonation increases interminably in time. Whilst the model proposed by Czarnecki and Woyciechowski (2012) and Woyciechowski *et al.* (2019) consider the saturation of pores with carbonation products, their formulation is yet limited. Also, an important difference between the analytical models and the ML model is the number of considered variables. The formulae reported by Sarja and Vesikari (1996) considered the highest number of variables and proposed a relation between the carbonation depth and the compressive strength. However, these considerations were not enough to determine accurately the carbonation depth of specimens different from those considered in their experimental study.

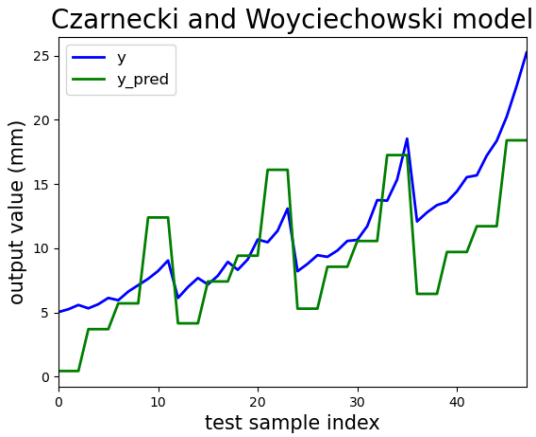

Figure 4-9: Actual and predicted values using the formulation proposed by Czarnecki and Woyciechowski (2012).

Table 4-6 reports the performance of the three empirical formulations considered to determine the carbonation depth. The Czarnecki and Woyciechowski (2012) model performed fairly as it achieved $RMSE$, MAE, and R^2 values of 3.692, 3.129 and 0.383, respectively. Both the formulae proposed by Woyciechowski *et al.* (2019) and the one reported by Sarja and Vesikari (1996) failed to predict the experimentally measured carbonation depth of the concrete experiments. Whilst the first achieved an $RMSE$ of 7.074, MAE of 4.052, and R^2 of -3.728, the second one obtained a $RMSE$, MAE, and R^2 values of 11.94, 11.069, and -3.756, respectively.

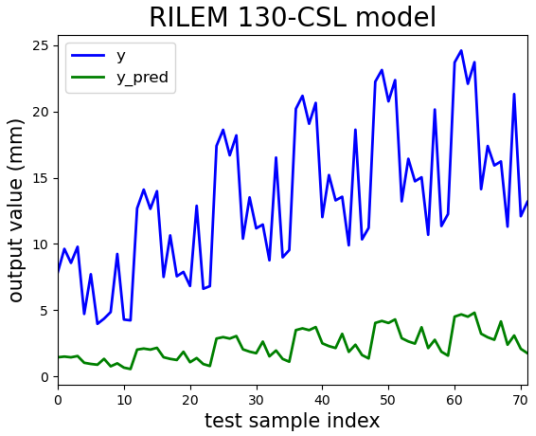

Figure 4-10: Actual and predicted values using the formulation found in the RILEM report edited by Sarja and Vesikari (1996).

Table 4-6: Performance of the analytical models to predict the carbonation depth

Model	Tested data	*RMSE*	*MAE*	R^2
RILEM 130-CSL model	72	11.944	11.069	-3.756
Czarnecki and Woyciechowski model	48	3.692	3.129	0.383
Woyciechowski et al. model	16	7.074	4.052	-3.728
Gradient boosting regression tree model	**214**	**1.514**	**0.905**	**0.971**

The discussion above emphasizes the importance of powerful marching learning algorithms in data mapping and classification in solving complex problems in materials science as well as other fields. While the three empirical models reported in the literature were strictly applied only to a small data set that mimics the specific conditions deployed in developing those models, they failed to predict experimental carbonation depth for data different from the samples used to develop their models. Conversely, the machine learning based GBRT model was applied to a comprehensive data set of 713 experimental results retrieved from the open literature. The diversity of the experiments did not prevent the GBRT model from achieving excellent performance in predicting the carbonation depth. Yet, it largely outperformed the accuracy of all the empirical models, despite that those models were applied to a small data set restricted to their specific requirements.

4.5 Conclusions

This study explored the potential use of a machine learning GBRT model to predict the carbonation depth of RAC containing different types of binders, such as metakaolin, silica fume, blast furnace slag and fly ash. For this purpose, 713 data-records were retrieved from the open literature, characterized by 17 attributes as input features. To further analyze the GBRT model thus developed, a feature importance analysis was performed. The predictive accuracy of the GBRT model was then compared to that of existing analytical formulations to determine the carbonation depth of concrete. From the formulation and analysis performed in the present study, several conclusions can be drawn:

- The GBRT model demonstrated exceptional performance in predicting carbonation depth. Over the 214 test samples not used in training and thus unfamiliar to the model, GBRT achieved a $RMSE$ of 1.5139, MAE of 0.948, and R^2 of 0.9707. The robustness of the built model was proven by the close scores obtained with the different random seeds.

- From the feature analysis, metakaolin, blast furnace slag, and silica fume did not manifest high impact on the carbonation resistance of concrete. However, scarce studies reported the inclusion of these type of binders. More research is needed to investigate further the inclusion of such binders.
- The attributes with the greatest influence on carbonation depth of concrete were found to be the compressive strength and the water-to-binder ratio, which is in concordance with other studies (R. V. Silva et al., 2015) since they reflect the pore structure of the cementitious matrix.
- The analytical models to determine the carbonation depth of concrete were found to be unsuitable for capturing this phenomenon, despite that they were applied to their restricted domain of development and data samples similar to that used to originate their formulation.

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Chapter 5

5 Conclusions, Recommendations and Future Research

5.1 Summary and Conclusions

The present research analyzed the feasibility of utilizing machine learning (ML) algorithms to model the performance of recycled aggregate concrete (RAC). The main objectives of this thesis have been to i) trace and analyze the application of ML methods to the prediction of compressive strength of modern concretes; ii) develop state-of-the-art ML models to predict the compressive strength of RAC using a large and diverse database; iii) perform and optimize RAC mixture design using a particle swarm optimization algorithm coupled with gradient boosting regression tree; and iv) predict the carbonation depth of RAC using ML techniques. In general, the application of ML methods demonstrated remarkable performance to determine the compressive strength and carbonation depth of RAC. In this chapter, the conclusions of the entire research are presented, along with recommendations and future research suggestions.

In the second Chapter, a critical survey of recent applications of machine learning techniques to predict the compressive strength of modern concretes was done. The complex mixture of non-conventional concretes did not hinder the ability of the different ML models to achieve accurate compressive strength predictions. From this review, it was concluded that the most widely applied ML technique to predict the compressive strength has been the artificial neural networks owing to its superior accuracy. However, the lack of clarity to forecast predictions of this type of models is considered a great disadvantage. Accordingly, other techniques have been explored. For instance, genetic algorithms are recommended if the purpose is to develop an equation that describes the compressive strength of modern concretes.

In Chapter three, an application of three different ML techniques was applied to predict the compressive strength of RAC: Gaussian processes, gradient boosting regression tree, and deep learning. The three models manifested extraordinary predictive performance. However, the deep learning and gradient boosting regression tree models revealed higher performance as they guaranteed appropriate generalization of the intrinsic principles to

predict the compressive strength of RAC. Also, the mixture optimization proposed in this chapter accomplished a significant reduction of mixture cost in most of the cases. Following the emerging sustainable requirements, it is of paramount importance to pursue the reduction of material volumes, and subsequently the reduction of costs, in concrete mixture design.

Chapter four presents the determination of carbonation resistance of RAC using ML techniques for the first time. The gradient boosting regression tree used in this chapter demonstrated extraordinary capability to determine the carbonation depth using 17 different attributes as input features. These features were principally related to the characterization of the mixture components. A feature analysis was then performed which identified the high influence of the compressive strength, water-to-binder ratio and exposure time to carbon dioxide on the carbonation resistance of the RAC mixtures. Subsequently, a comparison to other theoretical models was carried out emphasizing the need for more advanced techniques, such as the machine learning model developed herein.

5.2 Future Research and Recommendations

As mentioned earlier, one of the main objectives of ML techniques is to develop models that are able to generalize the phenomenon in question. Therefore, it is of great importance that the process of developing models to predict the properties of the different cementitious composites ensures the generalization capacity of ML methods.

Considering the stringent sustainable development needs in recent years, it is of paramount importance to intensify the utilization of by-products and recycled materials. The use of supplementary cementitious materials is one latent solution to decrease the carbon footprint generated by the production of cement. However, researchers still need to explore mixtures incorporating different types of supplementary cementitious materials or geopolymers along with recycled aggregates. Thus, further study is required on the effect of blast furnace slag, metakaolin, silica fume, other recycled materials, geopolymers and alkali-activated systems on the compressive strength of recycled aggregate concrete.

Similarly, in the carbonation resistance of recycled aggregate concrete, further studies are needed on the effect of other types of binders, such as metakaolin, blast furnace slag, and silica fume.

Also, most of the studies that aimed at creating analytical formulations to determine the carbonation depth of concrete developed their models based on a limited number of experimental samples. Thus, to ensure that the created models capture the phenomena unbiasedly, it is of great importance to carry out a diverse collection of experimental works.

It is of relevant significance to consider that machine learning applications will continue to grow, and that these techniques along with big data analysis, and the internet of things will govern the industrial world in the coming decades. The cement and concrete industries must adapt to this reality and benefit from the vast opportunities it presents.

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