Comparison of Different Data Mining Techniques for Predicting Compressive Strength of Environmentally Friendly Concrete

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Abstract: With its growing emphasis on sustainability, the construction industry is increasingly interested in environmentally friendly concrete produced using alternative and/or recycled waste materials. However, the wide application of such concrete is hindered by lack of understanding of the impacts of these materials on concrete properties. This research investigates and compares the performance of nine data mining models in predicting the compressive strength of a new type of concrete containing three alternative materials as fly ash, Haydite® lightweight aggregate, and Portland limestone cement. These models include three advanced predictive models (multilayer perceptron, support vector machines, and Gaussian processes regression), four regression tree models (M5P, REPTree, M5-Rules, and decision stump), and two ensemble methods (additive regression and bagging) with each of the seven individual models used as base classifier. The analytical results show that with appropriate parameter settings all of these models except for decision stump achieved acceptable prediction performance. The ensemble methods improved the prediction accuracy of the four regression tree models, but had less success on the other three advance predictive models. The individual Gaussian processes regression model as well as its related ensemble models reached the highest prediction accuracy in comparison groups. The results of this paper offer valuable insights to improving the use of these models for property prediction of concrete.

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Introduction

The construction industry has observed an increasing shift toward sustainability in recent years. Many companies are proactively using or are required by their clients to use more environmentally friendly (or so-called "green") building materials and/or processes to reduce the environmental effects from construction activities. Environmentally friendly concrete is defined as concrete produced using alternative and/or recycled waste materials that can lower the overall environmental impacts of concrete during its life cycle. This type of concrete increasingly becomes a common element that helps the construction industry achieve long-term sustainability, although the impact of these alternative or recycled waste materials on various concrete properties has not been fully understood.

Using alternative materials in concrete may positively or negatively impact its properties (Khalaf and Devenny 2004; Yang et al. 2005; Berry et al. 2011). Research is thus needed to thoroughly understand the potential influence from these materials. Since the compressive strength is one of the most important concrete properties, many experiments have been conducted to study the compressive strength of environmentally friendly concrete (Yang et al. 2005; Etxeberria et al. 2007; Kevern et al. 2011). Despite some progress, the available data for such concrete is far from adequate due to the emergence of so many alternative or recycled waste materials and the complexity of concrete mixture design. Not only is more research needed to advance the understanding of environmentally friendly concrete properties, but practical tools for designing these types of concrete are necessary for wide implementation.

Differing from the traditional experimental method, some researchers proposed mathematical or statistical models to predict the compressive strength of concrete given its mixture or based on fresh concrete properties (Atici 2011). Statistical modeling has its limitations in estimating the underlying relationships between the inputs and outputs of forecasting models in more complicated cases (Zhang 1998). As a result, recent studies have shown an increasing trend toward the application of machine learning techniques in predicting concrete compressive strength (Topçu and Saridemir, 2007; Saridemir et al. 2009; Atici 2011; Aiyer et al. 2014; Akande et al. 2014; Omran et al. 2014). The results from these studies demonstrate a great potential of this approach, which warrants further investigation.

The research presented in this paper compared the use of seven individual machine learning models, including M5Prime (M5P), REPTree, M5Rules, decision stump, multilayer perceptron, SMO regression (SMOreg), and Gaussian processes, in predicting the compressive strength of environmentally friendly concrete. It also tested two commonly used ensemble methods (additive regression and bagging) by adopting each of the seven individual models as the base classifier to explore the possibility of improving prediction accuracy. The ultimate goal was to promote the use of data mining techniques for determining the compressive strength or other properties of new types of concrete while reducing the need for extensive experiments. This shift will not only save time and money for the industry, but also facilitate the use of new materials. The unique set of seven data mining models was selected for exploring the prediction performance of four regression tree models against other three more advanced models. This also seemed to be the first time that Gaussian processes regression was examined for predicting concrete strength. This research used four performance measures, namely correlation coefficient (R), coefficient of determination (R^2), root mean squared error (RMSE), and mean absolute error (MAE), to assess prediction accuracy of generated models. R^2 was used to compare models examined in this research and previous studies.

This paper first introduces the unique type of environmentally friendly concrete studied in this research and then reviews previous research efforts in modeling and predicting compressive strength of concrete. A brief description of all the data mining models examined in this research is presented. After describing the research methodology and experimental settings, this paper presents the results and analysis as well as the findings of this research.

Literature Review

Environmentally Friendly Concrete

Conventional concrete is made from four main ingredients: water, cement, fine aggregate (sand), and coarse aggregate. With the wide use of concrete as a building material, its negative environmental impacts are significant. Specifically, the cement industry produces up to 5% of global man-made CO_2 emissions (WBCSD 2009) and accounts for approximately 12–15% of total industrial energy use in various countries (Madlool 2013). The concept of producing more environmentally friendly concrete emerged as a response to reducing the emissions and other environmental impacts from concrete production. For this purpose or as a result of a demand for specific properties needed for concrete applications, alternative materials (particularly supplementary cementitious materials [SCMs] and alternative aggregates) are added or used to replace certain amounts of the traditional ingredients.

For environmentally friendly concrete, the commonly used alternative materials are those that contain recycled contents, are locally available with low transportation costs, have reduced greenhouse gas emissions in their production, reserve natural resources, or improve concrete performance during its life cycle. Some of the frequently studied alternative aggregates include recycled concrete aggregate (Etxeberria et al. 2007; Limbachiya et al. 2012), building rubbles (Khalaf and Devenny 2004), fiber scrap aggregate (Shahria Alamet al. 2013), recycled glass aggregate (Berry et al., 2011), etc. Fly ash (FA) class C and F (Basri et al. 1999; Kevern et al.

2011), furnace slag (Lubeck et al. 2012), and silica fume (Limbachiya et al. 2012), are examples of materials that have been examined as SCMs.

For this research, Portland limestone cement (PLC), Haydite® lightweight aggregate (LWA), and FA Class F were selected as alternatives to the traditional ingredients. This was based on the literature review and the results of a survey that was performed by the research team to identify industry interests in using environmentally friendly concrete and ingredients (Jin 2013). A brief review of these alternative materials can be found in Omran et al. (2014).

Related Work in Modeling and Predicting Concrete Properties

The experimental determination of the compressive strength of concrete, especially for concrete containing alternative materials, is known to be time consuming and costly. On the other hand, using simple linear regression models for prediction has limited accuracy and flexibility (Yeh 1998; Deepa et al. 2010). As a result, recent years have seen an increasing interest in using more advanced data mining techniques for predicting concrete properties.

Artificial neural network (ANN) has been used to predict fresh and hardened properties of high performance concrete (Khan et al. 2013) and LWA concrete (Alshihri et al. 2009; Abdeen and Hodhod 2010). The results of these studies have generally confirmed ANN to be a powerful method for such applications. Another widely used data mining method, Support Vector Machines (SVM), has also been used to predict properties of hardened concrete, such as compressive strength, tensile strength, and elastic modulus (Gupta 2007; Yan et al. 2013; Yazdi et al. 2013; Aiyer et al. 2014; Akande et al. 2014). In other attempts, both ANN and SVM have been applied in conjunction with fuzzy logic to improve the accuracy and reliability of prediction (Nataraja et al. 2006; Saridemir et al. 2009; Cheng et al. 2012). In addition, some other prediction models, e.g., ensembles of decision trees in Erdal et al. (2013), were examined for predicting the compressive strength of different types of concrete. While these studies have led to more accurate predictions compared to traditional regression techniques, more reliable, applicable, and practicable models are yet to be discovered (Chou et al. 2011).

A comparison between multivariable regression analysis and ANN made by Atici (2011) identified the effectiveness of these methods for predicting the strength of mineral admixture concrete. With the increasing use of advanced data mining techniques in concrete property prediction, a few other comparison studies were conducted to evaluate the performance of multiple data mining models, mostly focused on the compressive strength prediction of high performance concrete. For example, Deepa et al. (2010) examined ANN, linear regression, and M5P tree model for their accuracy and time performance. Similarly, Chou et al. (2011) evaluated ANN, SVM, multiple regression, multiple additive regression trees, and bagging regression trees. So far, very few studies have compared multiple data mining methods in predicting the compressive strength of environmentally friendly concrete. This paper aims to fill this gap and provide a more accurate and reliable tool to predict the compressive strength of a unique type of environmentally friendly concrete made with PLC, Haydite LWA, and FA.

Predictive Data Mining Techniques Examined in This Research

The research was performed in two steps: 1) Examining the prediction accuracy of seven individual data mining models, including the four common regression tree models (M5P, REPTree, M5-Rules, and decision stump) and three more advanced predictive models (multilayer perceptron, SMOreg, and Gaussian processes regression), and 2) Examining the prediction accuracy of two commonly used ensemble methods (additive regression and bagging), in which each of the aforementioned models was used as base classifier to evaluate the effects of boosting. Kotsiantis et al. (2006) defined three mechanisms for the ensemble of regression models: 1) *using a single machine learning model with different subsets of training data*, 2) *using a single learning method with different training parameters*, and 3) *using different machine learning methods*. The second step of this research adopted the first two mechanisms by using a single machine learning model as base classifier for the ensemble models. Studying multiple classifiers for the ensemble models can be a subject for future research. A brief review of these data mining models and selected parameters is presented below.

Regression Tree Models

Regression tree models have long been used in data mining as a supervised learning technique, and have been widely applied to numeric prediction. Compared to some of the state-of-the-art models, regression tree models may have lower prediction accuracy, but usually perform faster and are easier to interpret. This research examined four commonly used regression tree models as described below.

M5P is a reconstruction of the M5 algorithm introduced by Quinlan (1992) for generating a tree of regression models from empirical data (Wang and Witten 1997). In a M5P model, at each branch the tree stores a linear regression model that predicts the class values of the portion of dataset that reaches the leaf. The dataset splits into different portions according to certain attributes of the data. Standard deviation (SD) is usually used as a criterion that determines which attribute is the best for splitting the dataset at each node. The attribute to be chosen is the one that has the maximum expectation to reduce error, see Eq. (1):

$$EX_{error} = SD(T) - \sum \frac{|Ti|}{|T|} \times SD\ (T_i) \qquad (1)$$

where T_i denotes the subset of cases that have the ith outcome of the potential test. The process stops when a very small change happens in class values or only a few instances remain. The tree will then be pruned back and a smoothing process will be performed in the end to compensate sharp discontinuities between adjacent linear models (Quinlan 1992).

REPTree (Reduced Error Pruning Tree) is a fast decision tree learner that builds a decision/regression tree by using information gain or variance as decision features for splitting the data at the nodes. Then the generated regression tree is pruned back using the reduced-error with back over-fitting technique (Witten and Frank 2005). In the context of decision trees, the term "information gain" is usually equivalent to expectation value of the Kullback–Leibler divergence of a conditional probability distribution (Garcia et al. 2002). For numeric attributes, REPTree sorts the values once at the start of the run, and then uses the sorted list to calculate the right splits in each tree node.

M5-Rules is an algorithm that uses divide-and-conquer to generate decision lists (ordered sets of if-then rule) for regression problems. Holmes et al. (1999) used decision lists to make a more compact and understandable model tree compared to previous models. Decision lists can work with both continuous and nominal variables. M5-Rules uses the M5 algorithm to build a model tree, makes a rule from the best leaf, and then works on other instances that are left in the dataset according to the generated rule.

Decision Stump is a machine learning model that only consists of one-level decision tree. It has one internal node (called root node), which is immediately connected to nodes in branches (referred to as terminal nodes). Decision stump makes a prediction based on the value of just a single input attribute. It performs regression based on the mean squared error where each root node represents an attribute in an instance to be evaluated, and each branch represents a value that the node can take (Iba and Langley 1992). Decision stump is usually used as a component of a boosting algorithm to improve its prediction accuracy.

Multilayer Perceptron (ANN)

ANN is a computational system consisting of simple, highly interconnected processing elements (nodes or neurons) that work together to solve specific problems (Caudill 1987). It is an algorithm inspired by research in biological nervous systems to generate a simplified model of how the brain works (Rumelhart et al. 1994). The first neural network was proposed by McCulloch and Pitts (1943), and since then many other models have been introduced. The basic structure of a multilayer perceptron ANN model is shown in Fig. 1 below.

ANN models usually consist of an input layer, one or more hidden layers, and an output layer. Each of these layers can have different number of nodes. Each node under the hidden layer(s) will receive one or more inputs. The inputs will be multiplied by their weights, and summed together and with the bias (threshold). The weighting and bias values will be initially chosen as random numbers and will then be adjusted according to the results of the training process (Atici 2011). The output of each node will be generated based on the significance of the summation value and by the means of a predefined specific activation function, e.g., unipolar sigmoid function, bipolar sigmoid function, hyperbolic tangent function, etc. (Bishop 2006).

SMOreg-based SVM

SVM is a supervised learning model developed by Cortes and Vapnik (1995). It has been intensively used in many data mining problems for both classification and regression purposes. In an SVM algorithm, the training set is first mapped to an n-dimensional feature space by using a nonlinear kernel mapping procedure. Then a hyperplane, a subspace that is one dimension less than its surrounding space, will be identified in this feature space according to the projected dataset. The aim is to find the optimal hyperplane that separates the data points in the classes, while simultaneously maximizing the margin (i.e., the distance between the hyperplane and the closest points of the training set) for linearly separable patterns (Leskovec et al. 2014). The hyperplane $f(x, w)$ is represented by a linear function in the feature space:

$$f(x, w) = \sum_{j=1}^{m} w_j \, g_j(x) + b \qquad (2)$$

where $g_j(x)_{,j=1,\dots,m}$ denotes a set of nonlinear transformations, and *b* is the "bias" term. For SVM regression purposes, Cortes and Vapnik (1995) suggested to use a so called ε, the insensitive loss function that penalizes error only if it is greater than ε (Shevade et al. 2000). So the $|\xi|_\varepsilon$ is represented as:

$$|\xi|_\varepsilon = \begin{cases} 0 & if\ |\xi| \leq \varepsilon \\ |\xi| - \varepsilon & otherwise \end{cases} \qquad (3)$$

Using (non-negative) slack variables ξ_i and $\xi_i{}^*$, the final optimization problem to be solved can be formulated as:

$$\text{Minimize} \quad \frac{1}{2}\left||w|\right|^2 + C \sum_{i=1}^{l} (\xi_i + \xi_i{}^*) \qquad (4)$$

Subjected to:

$$\begin{cases} y_i - f(x_i, w) \leq \varepsilon - \xi_i{}^* \\ f(x_i, w) - y_i \leq \varepsilon - \xi_i \\ \xi_i, \xi_i{}^* \geq 0, i = 1, \dots, n \end{cases} \qquad (5)$$

SVM regression finds the linear regression in the high-dimension feature space using ε while reducing the model complexity by minimizing $\left||w|\right|^2$.

Sequential minimal optimization (SMO), an algorithm introduced by Platt (1998), is used to solve the very large quadratic programming (QP) optimization problems in SVM through breaking them into a series of smallest possible QP problems. In this way problems can be solved analytically, eliminating the need for numerical optimization algorithms (Platt 1998).

Gaussian Processes

Gaussian process is a powerful non-linear prediction tool, which can be used for Bayesian regression as well as in learning process of both supervised and unsupervised learning frameworks (Bishop 2006). It is a non-parametric stochastic process that generalizes the Gaussian probability distribution. A Gaussian process sometimes is described as a distribution over functions ($P(f)$), where f is a function that projects input space (vector $\mathbf{x}$) to feature space (vector $\mathbf{r}$) and for any finite subset of X the marginal distribution over that subset $P(f)$ has a Gaussian distribution. The f could be an infinite-dimensional quantity. As a result, Gaussian process extends multivariate Gaussian distributions to infinite dimensionality (Rasmussen and Williams 2006). Same as Gaussian distribution that can be specified by a mean vector $\boldsymbol{\mu}$ and covariance matrix $\sum$, a Gaussian process can be defined by a mean function $M(x)$ and covariance function $k(x, x')$ expressed as $f(x) \sim GP\big(M(x), k(x, x')\big)$. One of the advantages of a Gaussian process model is that its formulation is probabilistic. This is especially useful for probabilistic prediction and "gives the ability to infer model parameters such as those that control the kernel shape and the noise level" (Chu and Ghahramani 2006).

Ensemble Methods Used in This Research

According to Rokach (2010), the idea of ensemble learning models started with Tukey (1977) at late 1970s by simply combining two linear regression models using residual of the first model for the second modeling process. This effort was then followed by many other attempts, such as partitioning the input space and using two or more classifiers (Dasarathy and Sheela 1979) or using the AdaBoost algorithm (Freund and Schapire 1996). The purpose for ensemble modeling is to achieve better prediction performance by combining multiple learning algorithms.

Additive Regression (Gradient Boosting)

Regression trees are well known for many advantages such as flexibility of input variables (e.g., numeric, ordinal, binary, and categorical variables) and immunity to the effects of extreme outliers. However, these methods usually suffer from the lack of accuracy. Gradient boosting, first introduced by Friedman (2001), is an additive regression tree model that can overcome this drawback through the application of a boosting technique (Friedman and Meulman 2003). Additive models are nonparametric regression methods, which assume that each input feature has a separate contribution to the final prediction and these input features can be added up to generate the regression model for prediction (Friedman and Stuetzle 1981). According to Friedman and Meulman (2003), boosting a tree-based model can significantly increase its prediction accuracy. Additive regression is a metadata learner that improves the performance of weak prediction models (e.g., regression tree models) by applying the stochastic gradient boosting technique. The technique mainly involves fitting sequence of models: The first model in the sequence is trained based on the original dataset, and each of the next models will be trained on a new dataset containing the residual errors remained from fitting the previous model (Friedman, 2001).

Bagging

Bagging is short for Bootstrap Aggregating. Breiman (1994) defines bagging as a way to generate multiple versions of a predictor, through which a more robust predictor can be generated. It is an ensemble meta-algorithm that improves the accuracy and stability of the prediction. The algorithm is based on generating bootstrap replications of dataset and using these different versions of dataset as new training sets to generate multiple models. The final prediction is achieved through combining the outcomes of these models (i.e., averaging the results for the regression problem and using plurality voting for the classification problem). Previous studies have shown that bagging can significantly improve the results of unstable models (e.g., models sensitive to small changes in the training dataset), models with high dimensional dataset problems, and classification and regression tree models (Breiman 1994; Buhlmann and Yu 2002).

Methodology and Experimental Settings

Concrete Experimental Design and Data Collection

In this study, 36 different batches of concrete were designed and prepared. Each batch contained different replacement percentages of fly ash Class F (0%, 20%, 30% or 40%) and Haydite LWA (0%, 33%, 67% or 100%) besides the use of either Portland cement (PC) Type I/II or PLC Type GUL. In this way, the effects of alternative materials on the compressive strength of concrete can be examined more accurately. The fly ash Class F replaced part of PC or PLC by different percentages of weight and Haydite LWA substituted pea gravel by different percentages of volume. Their numerical values were used as inputs for the tested models. In addition to the above three variables, the actual water content, the amounts of sand, pea gravel, and Micro Air®, as well as the concrete curing age were selected as the other influential variables for the models. Table 1 shows the range, mean, and SD of those variables in this experimental study.

All the concrete mixed in the experiment was assumed to be air-entrained (considered to be used outdoors in cold climate) by adding Micro Air, an air entraining agent, to the mixtures. The intended slump was 12.70 - 15.24 cm and the air content was 6-7%. Concrete was mixed in a laboratory mixer and the whole processes of making, pouring and curing concrete were performed based on ASTM C 31/C 31 M – 06 guideline. Three 10.16 cm by 20.32 cm cylinders from each batch of concrete mixture were tested in each of four different curing ages of 3, 7, 28 and 90 days for compressive strength. The average test result of each three cylinders formed a data point in the database. All the details for the experiments can be found in Jin (2013).

Parameter Setting of Data Mining Models

In this study, the Weka workbench toolbox (Waikato 2015) was used to generate the examined machine learning models for predicting the compressive strength of the environmentally friendly concrete. Since one of the original goals for experimental testing was to compare the compressive strength of PC and PLC concrete, this research performed a simple paired T-Test on the PC and PLC concrete datasets, which confirmed a statistical difference between these two groups. To evaluate the potential impact of the statistically different datasets on the prediction accuracy of data mining models, this research took the following three-step approach: The first was to test the selected data mining models based on the PC or PLC dataset only. In such cases, seven variables were used to generate the models. The second step was to examine the selected models based on the whole dataset including all PC and PLC concrete samples. In the modeling process, eight variables including a new binary variable "cement type" were used. Thirdly, the prediction performance of data mining models based on different datasets was compared to learn whether simpler models with seven variables and individual datasets will lead to better prediction accuracy, or the prediction accuracy can be improved by a larger sample size though additional variable(s) may be needed, leading to more complex models.

An example of ANN model with eight input variables including "cement type" is shown in Fig. 2. The symbol "8-3-1" means that there are eight nodes in the input layer, three nodes in the hidden layer, and only one node at the output of the network.

Many input parameters need to be set up for most data mining algorithms. The setting of input parameters could affect the accuracy and/or reliability of generated models. In this research, a comprehensive sensitive analysis was carefully conducted on each model to identify the parameter values/options that could lead to the highest prediction accuracy among all the examined model settings, while avoiding over-fitting issues. The important parameters that were tested in this sensitivity analysis are presented in the Analytical Results and Discussion section.

Performance Measures

The models were trained with different parameters and/or variables. Their prediction accuracy was evaluated and compared based on four frequently used performance measurements in previous studies: R, R^2, RMSE, and MAE. R, RMSE, and MAE are formulated as:

$$\mathrm{R} = \frac{\sum_{i=1}^{n}(P_i - \mu_P)(A_i - \mu_A)}{\sqrt{\sum_{i=1}^{n}(P_i - \mu_P)^2}\ \sum_{i=1}^{n}(A_i - \mu_A)^2} \tag{6}$$

$$\mathrm{RMSE} = \sqrt{\frac{\sum_{i=1}^{n}(P_i - A_i)^2}{n}} \tag{7}$$

$$\mathrm{MAE} = \frac{\sum_{i=1}^{n}|P_i - A_i|}{n} \tag{8}$$

where A_i and P_i represent the actual and predicted compressive strength of concrete samples related to data point *i*, respectively, *n* is the total number of data points in the validation set(s), μ_A is the mean value of observations, and μ_P is the mean value of predictions.

A 10-fold cross-validation was used in this study to minimize the bias associated with the random sampling of the training and holdout data samples in regular validation methods. The cross-validation is a technique that evaluates the expected accuracy and validity of a predictive model by dividing a dataset into different subsets and evaluating the accuracy of the model for each of those subsets. In general, a k-fold cross-validation includes the following steps:

- Splitting the dataset into K subsets of equal size (K folds)
- In each run, training the model on all the subsets except one
- Evaluating the prediction accuracy by using the left out subset to test the trained model
- Repeating steps 2 and 3 for K times and each time leaving a different fold for testing
- Calculating the final performance measurements by averaging the performance

measurements from each of the K runs.

This would improve the generalization and reliability of the performance measurements obtained for models under testing.

Analytical Results and Discussion

Characteristics of Concrete Datasets Used in This Research

The datasets used in this research, i.e., the measured compressive strength of PC and PLC concrete samples, are illustrated in Fig. 3. It can be noted that the dramatic changes in compressive strength values shown in the figure were caused by different curing ages of the tested samples (3, 7, 28, and 90 days). The variation of compressive strength values obtained at the same curing ages was caused by different concrete mix designs.

Table 2 shows the results of the paired T-Test, which suggest that a statistically significant difference exists between the average compressive strength of PC- and PLC-based concrete. In other words, it shows that with 95% confidence, the average compressive strength of PLC concrete samples is 2.76 to 4.36 MPa higher than that of PC concrete samples.

Comparison Results for the Data Mining Models Tested

In the following, comparison results for the data mining models tested in this research are presented. Due to its poor prediction accuracy (e.g., R values at 0.5226, 0.6001 and 0.6208 for the PLC, PC and combined datasets, respectively), the decision stump model is excluded from most of the tables and figures presented below. The exception is for the presentation of results related to ensemble models. This is because this study found that when decision stump was used as the base classifier for the ensemble models, the prediction accuracy was acceptable.

Fig. 4 shows the highest R achieved by each of the eight data mining models. It was found that the prediction accuracy increased in five of the tested models when combining the two datasets (PC and PLC) and using the cement type as an additional binary input. Exceptions are the three regression tree models (i.e., M5P, REPTree and M5-Rules), in which the accuracy of prediction based on the PC concrete dataset was slightly better than the combined dataset.

The measured performance of prediction models in terms of RMSE and MAE is presented in Tables 3 and 4. The bolded value in each row represents the highest prediction accuracy achieved in this study when different datasets were used for testing individual and ensemble models. It seems that according to both criteria (MAE and RMSE), additive regression based on the Gaussian processes classifier obtained the highest prediction accuracy for comprehensive strength of PLC samples while the individual Gaussian processes regression model achieved the highest prediction accuracy for both the PC and combination datasets.

The information presented above shows that the listed models all had acceptable prediction performance. Further, the Gaussian processes regression model achieved the best prediction accuracy based on all the three performance measures while REPTree had the lowest. Table 5 below lists the important parameters and associated values/options used for these models to achieve their highest prediction accuracy. In particular, the option of "polykernel" was selected for all of the four models that need a kernel as their covariance matrix. These include additive regression, bagging, Gaussian processes, and SMOreg. From this point forward, the analysis and results are solely presented for the combined (PC & PLC) dataset, which was proven to have improved the prediction accuracy for most models tested in this study.

Fig. 5 illustrates the relationship between the predicted and actual compressive strength of the studied concrete samples for each of the eight predictive models. All the plots show fairly linear relationships between predicted and actual values. Apparently, the Gaussian processes regression model is the best representative of actual experimental data with the highest R^2 at

0.9842.

Fig. 6 displays the distribution of residuals and percentage error for the tested models. It is observed that in all these plots when the actual compressive strength of concrete samples increased, residuals became larger but the associated percentage errors decreased. Similar to the early findings, Gaussian processes regression, bagging, and additive regressions are the models with prediction results being the closest to the actual experimental values.

Table 6 compares R values achieved by the seven individual data mining models as well as two ensemble methods with each of individual data mining models used as base classifier. The comparison results show that both the additive regression and bagging algorithms using regression tree models as base classifier achieved better prediction accuracy than individual regression tree models. On the other hand, when SMOreg, Gaussian processes, and multilayer perceptron were used as base classifier, mixed results were generated. Similar to the early conclusion from the individual model comparison, the highest accuracy of prediction for additive regression and bagging was all achieved when the Gaussian processes was used as their base classification model. This finding is particularly important since Gaussian processes regression has rarely been applied in existing research to predict concrete properties.

Table 7 lists the average time spent for building each of the tested models. These times were associated with the parameter settings for these models to achieve the highest prediction accuracy in the sensitivity analysis. Due to the use of 10-fold cross validation, the training time for each of these models was much longer than the time used to build the model. Although many variables could affect the length of the training time, the total time was mostly proportional to the time used to build the model. The results indicate that even though the three more advanced predictive models achieved higher prediction accuracy in general they are far more time-consuming compared to individual regression tree models as well as ensemble models with regression tree as base classifier. The individual Gaussian processes model was somewhat an exception with relatively fast building and training time.

Comparison with Previous Work

Table 8 provides a brief comparison of the highest prediction performance achieved in this study and some of the primary previous works that used data mining models to predict the compressive strength of concrete. The comparison of R^2 values obtained by different studies shows that eight of the data mining models examined in this research offered fairly high prediction accuracy with R^2 ranging from 0.9217 to 0.9842. Moreover, compared with the same types of models examined in previous research, i.e., M5P, SVM, bagging, and additive regression, this study achieved relatively better prediction performance. It is worth noting that this research applied the cross validation method for evaluating the accuracy of predictions, which was not the case in most of previous studies listed in Table 9 except for Chou et al. (2011) and Deepa et al. (2010). Compared to the traditional validation method, cross validation usually lowers the R^2 values of tested models, but improves the generalization and reliability of the assessment.

According to Table 8, the Gaussian processes regression model provided the highest prediction accuracy (R^2 = 0.9837) among all the data mining models compared, while having a relatively fast modeling speed. Based on the extent of literature review performed by the authors, this research seemed to be the first work that examined Gaussian processes regression for predicting concrete properties, suggesting a great need for future research. Further, in most cases, ANN led to higher prediction accuracy than traditional modeling approaches such as linear regression or regression tree models.

In this research, the additive regression model would rank first in prediction accuracy when without the presence of Gaussian processes regression, which is consistent with the results from Chou et al. (2011). However, Chou et al. used decision stump as base classifier; this research found that additive regression based on decision stump had the lowest accuracy and the other six tested base classifiers could improve the prediction performance of additive regression. Also, in Chou et al. (2011), the prediction performance of bagging with the base fast decision tree leaner was not as good as the ANN model. In contrast, this study found that bagging could provide better prediction accuracy than the ANN model when using the advanced methods (i.e., Gaussian processes regression and multilayer perceptron) as base classifiers.

Conclusions

This research aimed to evaluate the potential of using data mining techniques for predicting the compressive strength of environmentally friendly concrete containing fly ash, Haydite LWA, and/or PLC. In particular, four common regression tree models (M5P, REPTree, M5-Rules, and decision stump) and three more advanced predictive models (ANN based on multilayer perceptron, SMOreg-based SVM regression, and Gaussian processes regression) were generated and tested individually. Then they were used as base classifiers in two ensemble models (additive regression and bagging) to evaluate the effects of boosting.

The obtained analytical results suggest that all of the tested models, except for decision stump, can provide acceptable prediction accuracy with R^2 ranging from 0.9217 (for REPTree) to 0.9842 (for Gaussian processes regression). The Gaussian processes regression model showed the best prediction accuracy as an individual data mining model. Also, when used as base classifier, it helped the two ensemble models achieve the best prediction performance. This observation is important since the Gaussian processes regression model is rarely investigated in previous works in this field.

The results of this research also indicate that in most cases, except for M5P, REPTree, and M5-Rules, training the models with the combined dataset containing PC and PLC concrete samples provided better prediction accuracy than using only the PC or PLC dataset. Furthermore, although the prediction accuracy of the three advanced data mining models was higher than that of the four regression tree models, the time required for building and training the models was significantly longer. This should be considered a factor in choosing an appropriate data mining model in practice. Particularly, when dealing with a very large dataset, using an ensemble method with a regression tree base classifier seems to be a more practical alternative. With the demonstrated potential of using data mining models to predict concrete comprehensive strength, future research can adopt this approach to study other properties of concrete such as tensile strength, durability, or concrete slump.

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Table List

Figure List

Table 1. Parameters and Values for Concrete Mix Design (Per Cubic Meter of Concrete)

Parameter	Min.	Max.	Mean	SD
Age (day)	3	90	35.12	35.37
Water (kg)	210.61	210.61	210.61	0
PC or PLC (kg)	226.63	528.02	346.18	102.07
Fly ash (kg)	0	211.21	79.80	72.37
Sand (kg)	741.60	901.78	768.29	59.91
Pea gravel (kg)	0	750.49	483.40	229.54
Haydite (kg)	0	368.42	131.13	113.03
Micro Air (ml)	112.17	135.38	123.78	11.64

Table 2. Paired T-Test of the Means for PC and PLC Concrete

Statistical item	Compressive strength for PLC concrete (MPa)	Compressive strength for PC concrete (MPa)
Mean	37.109125	33.54779
Variance	227.65862	195.3950
Observations	72	72
Hypothesized mean difference	0	
t stat	8.8572	
p(T<=t) one-tail	2.16E-13	
t critical one-tail	1.6665	
p(T<=t) two-tail	4.31E-13	
t critical two-tail	1.9939	

Table 3. The Lowest MAE Calculated for Each of the Models based on Different Datasets

Method	Additive Regression	Bagging	M5P	REPTree	M5-Rules	SMOreg	Multilayer Perceptron	Gaussian Processes
PLC	**1.52**	2.1038	3.4854	4.9203	3.9587	2.4839	1.946	1.6343
PC	1.8992	1.9536	2.4113	3.0505	2.3633	2.36	2.1796	**1.8784**
PLC & PC	1.3976	1.5662	2.4536	3.3953	2.4793	2.072	1.9625	**1.3756**

Table 4. The Lowest RMSE Calculated for Each of the Models based on Different Datasets

Method	Additive regression	Bagging	M5P	REPTree	M5-Rules	SMOreg	Multilayer perceptron	Gaussian processes
PLC	**2.0309**	2.6724	4.7615	6.2041	5.2028	3.3491	3.1178	2.2236
PC	2.4223	2.4563	2.9852	3.8477	2.9705	2.9571	2.9439	**2.4154**
PLC & PC	1.8624	1.9902	3.3367	4.1663	3.3169	2.6104	2.5473	**1.837**

Table 5. Important Parameters and Associated Values/Options for Achieving the Highest Accuracy of the Tested Models

Data mining model	The highest R	Name of parameter/option	Associated value/option
Additive regression	0.9918	Base classifier	Gaussian process
		Number (no.) of iteration	10
		Shrinkage rate	1
		Level of Gaussian noise	0.002
		Kernel of the choice	polykernel
		Exponent value	3
Bagging	0.9907	Base classifier	Gaussian process
		No. of iteration	80
		Bagging size percentage	100
		Level of Gaussian noise	0.007
		Kernel of the choice	polykernel
		Exponent value	3
M5P	0.9735	Min. no. of instances	5
M5-Rules	0.9738	Min. no. of instances	4
REPTree	0.9601	Min. total weight of instances	1
		Min. proportion of the variance	0.0001
SMOreg	0.9839	Kernel of the choice	polykernel
		Exponent value	3
Multilayer perceptron	0.9849	Node No. for first hidden layer	15
		Node No. for second hidden layer	8
		Learning Rate	0.1
		Momentum	0.25
		Training time	10000
		Validation threshold	20
Gaussian processes regression	0.9921	Kernel of the choice	polykernel
		Exponent value	3
		Level of Gaussian noise	0.0005

Table 6. R Values for Ensemble Models Using Different Classifiers

Method	REPTree	M5-Rules	M5P	Decision stump	SMOreg	Gaussian processes	Multilayer perceptron
Individual model	0.9601	0.9738	0.9735	0.6208	0.9839	**0.9921**	0.985
Additive regression	0.9822	0.9778	0.9917	0.9712	0.9845	**0.9918**	0.9793
Bagging	0.9701	0.9765	0.9786	0.9421	0.9823	**0.9907**	0.9899

Note: The bold numbers indicate the best performance result for each dataset.

Table 7. Time (in Second) for Building Each Model

Method	REPTree	M5Rules	M5P	Decision stump	SMOreg	Gaussian processes	Multilayer perceptron
Individual model	0.02	0.14	0.05	0	10.19	0.33	42.46
Additive regression	0.03	0.42	1.92	0.17	43.82	3.26	167.36
Bagging	0.28	1.09	3.71	0.03	127.02	27.89	419.42

Table 8. Comparison of Prediction Accuracy with Previous Works

Previous work	Sample size	Technique	R^2
Yeh 1998	727	ANN	0.914 (avg.)[a]
		Linear regression	0.574 (avg.)[a]
Gupta et al. 2006	864	Neural-fuzzy inference system	0.76
Fazel Zarandi et al. 2008	458	Fuzzy polynomial neural networks	0.8209
Yeh and Lien 2009	1196	Genetic operation trees	0.8669
		ANN	0.9338
Chou et al. 2011	1030	ANN	0.9091
		Multiple regression	0.6112
		SVM	0.8858
		Multiple Additive Regression Trees (MART)	0.9108
		Bagging Regression Trees (BRT)	0.8904
Deepa et al. 2010	300	Multilayer perceptron (ANN)	0.625
		Linear regression	0.491
		M5P model tree	0.787
Atici 2011	135	ANN	0.9801
		Multiple regression	0.899
Erdal et al. 2013	1030	ANN	0.9088
		Bagged ANN	0.9278
		Gradient Boosted ANN	0.9270
		Wavelet Bagged ANN	0.9397
		Wavelet Gradient Boosted ANN	0.9528
This paper	144	M5P model tree	0.9476
		M5-Rules	0.9482
		REPTree	0.9217
		Multilayer perceptron (ANN)	0.970
		SMOreg (SVM)	0.968
		Gaussian processes regression	0.9843
		Additive regression	0.9837
		Bagging	0.9816

[a]In Yeh (1998), the database was divided into four different sets. Each time one set was used for testing and the other three sets were used for training. The listed R^2 value is the average for the four testing datasets.

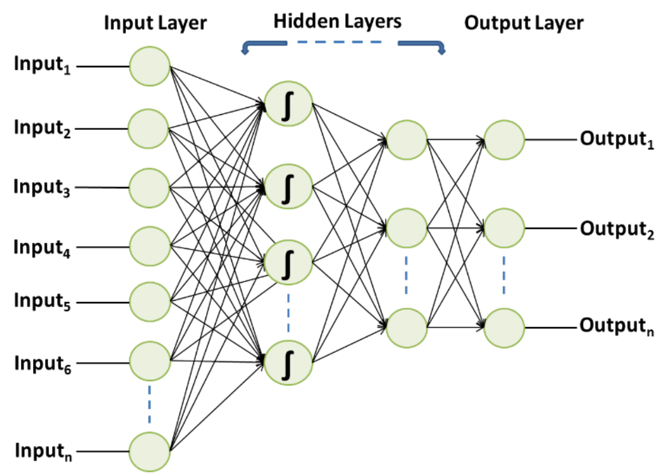


Fig. 1. Structure of ANN models

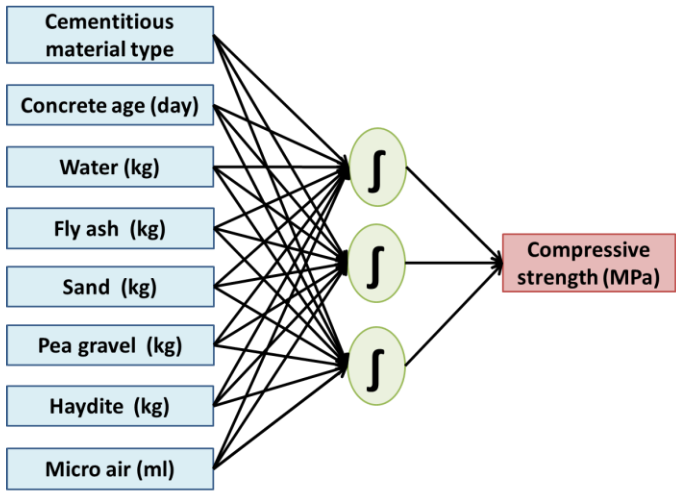


Fig. 2. The example ANN model (8-3-1)

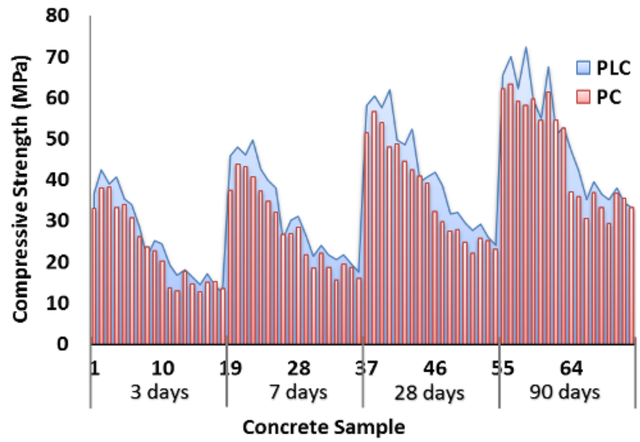
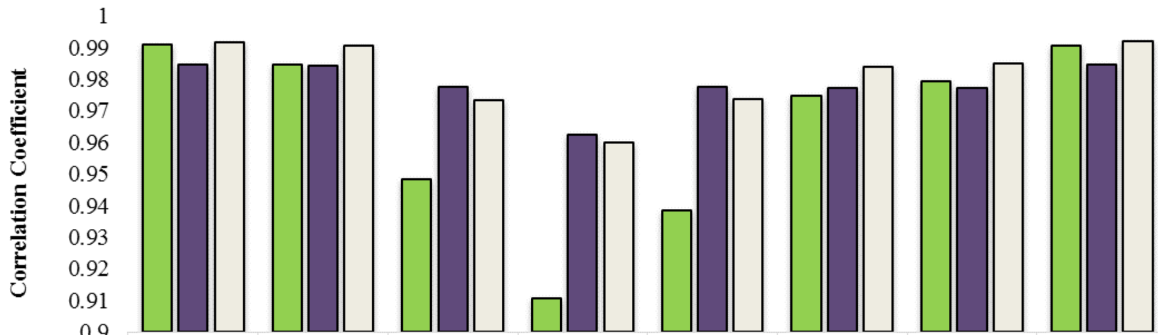


Fig. 3. Experimental results for compressive strength of PC and PLC concrete



	Additive Regression	Bagging	M5P	REPTree	M5Rules	SMOreg	Multilayer Perceptron	Gaussian Processes
PLC	0.9909	0.9845	0.9482	0.9105	0.9385	0.9748	0.9795	0.9907
PC	0.9847	0.9843	0.9775	0.9623	0.9774	0.9772	0.9773	0.9847
PLC & PC	0.9918	0.9907	0.9735	0.9601	0.9738	0.9839	0.985	0.9921

Fig. 4. The highest R value for each of the models based on different datasets

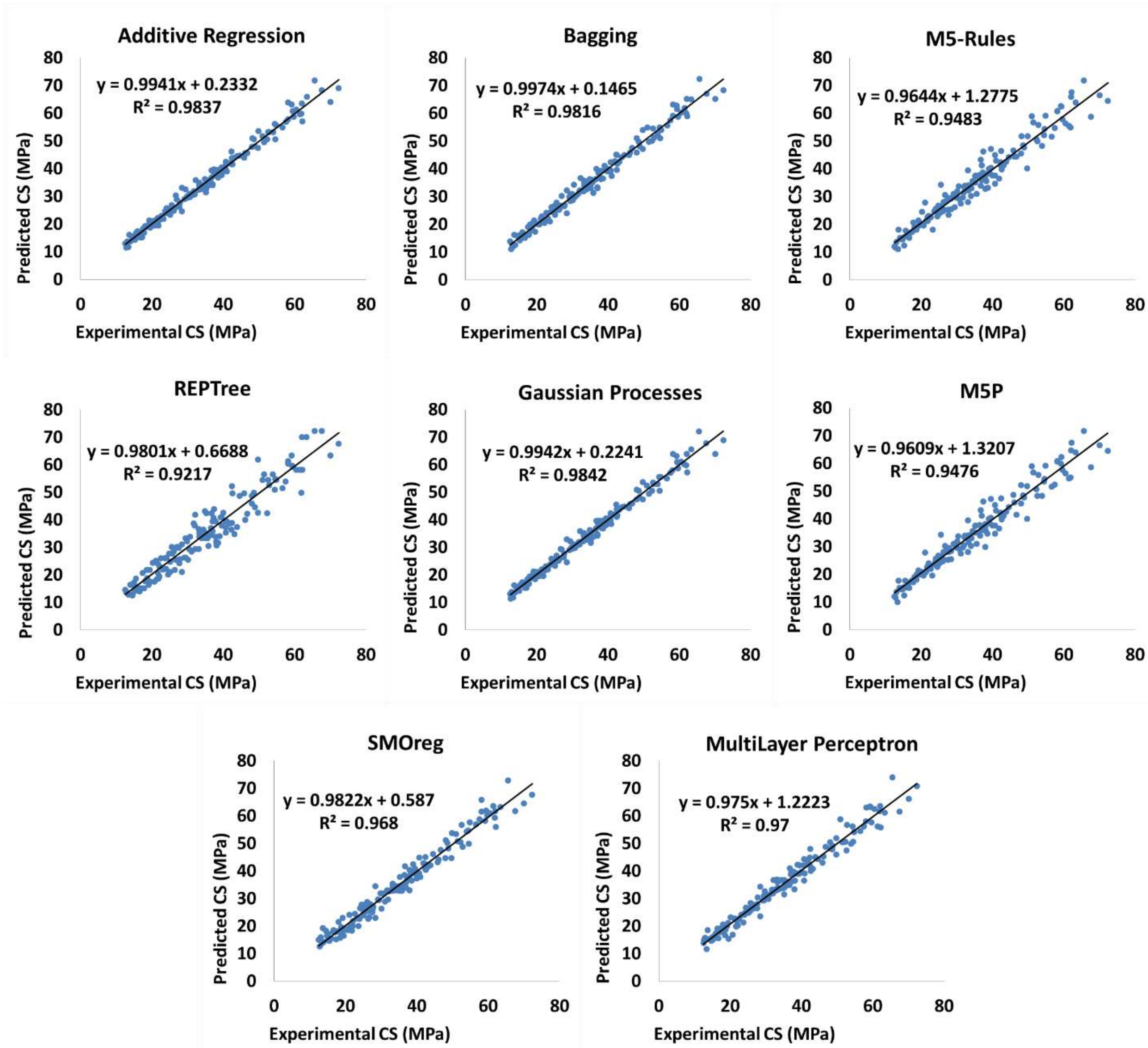


Fig. 5. Predicted vs. actual compressive strength (abbreviated as CS in the figure)

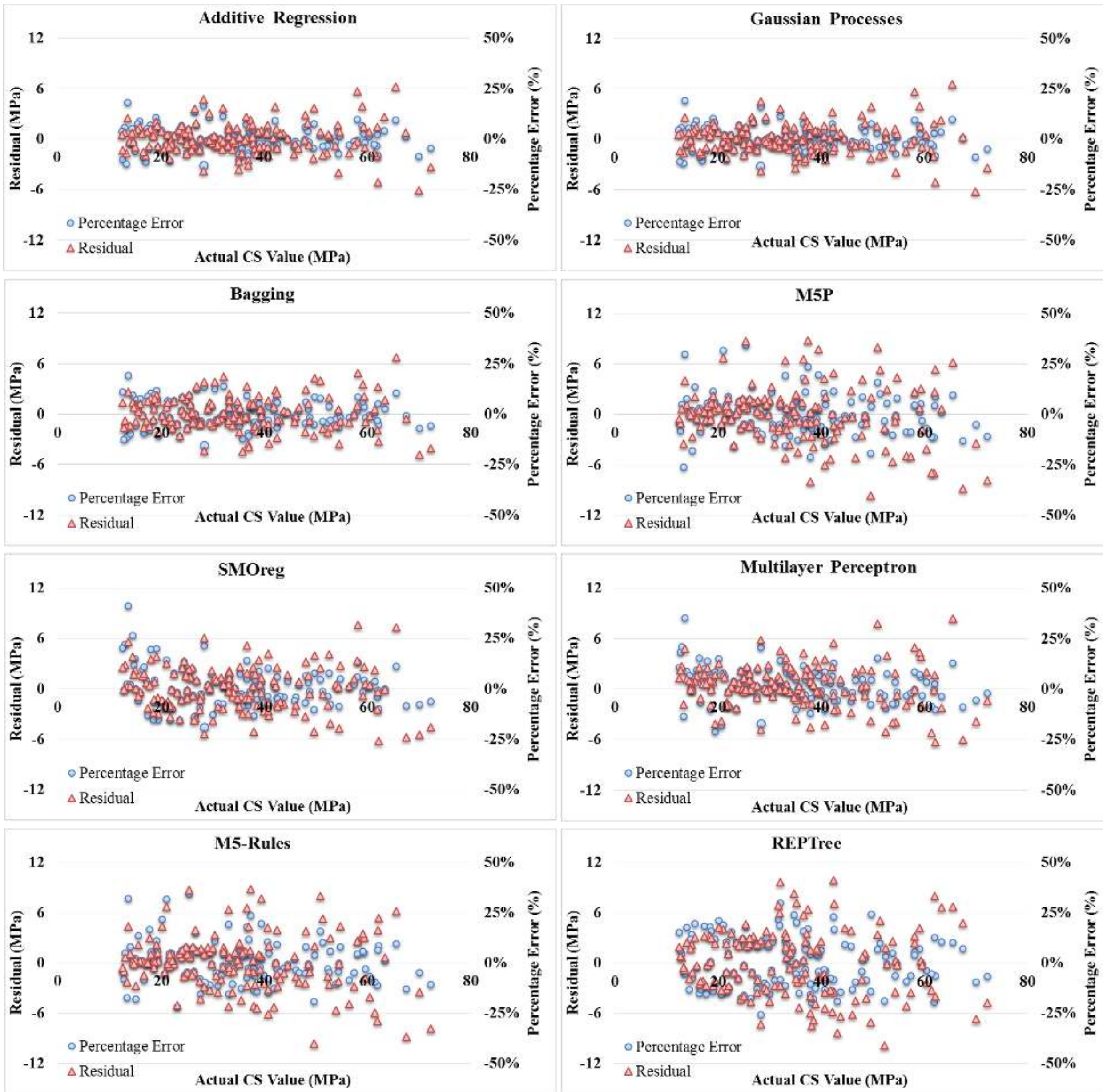


Fig. 6. Residuals and percentage errors vs. actual compressive strength values

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1. Estimating Length of Text

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1-column table = up to 60 characters wide by:	**2-column table = 61 to 120 characters wide by:**
17 lines (or less) = 158 word equiv.	17 lines (or less) = 315 word equiv.
up to 34 lines = 315 word equiv.	up to 34 lines = 630 word equiv.
up to 51 lines = 473 word equiv.	up to 51 lines = 945 word equiv.
up to 68 text lines = 630 word equiv.	up to 68 text lines = 1260 word equiv.

C. Total Characters wide by Total Text lines = word equiv. as shown in the table above. **Add word equivalents** for each table in the column labeled "**Word Equivalents.**"

3. Estimating Length of Figures

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1-column fig. = up to 3.5 in.(88.9mm)	2-col. fig. = 3.5 to 7 in.(88.9 to 177.8 mm) wide

C. Then use a ruler to check the height of each figure (including title & caption).

1-column fig. = up to 3.5 in.(88.9mm) wide by:	**2-column fig. = 3.5 to 7 in.(88.9 to 177.8 mm) wide by:**
up to 2.5 in.(63.5mm) high = 158 word equiv.	up to 2.5 in.(63.5mm) high = 315 word equiv.
up to 5 in.(127mm) high = 315 word equiv.	up to 5 in.(127mm) high = 630 word equiv.
up to 7 in.(177.8mm) high = 473 word equiv.	up to 7 in.(177.8mm) high = 945 word equiv.
up to 9 in.(228.6mm) high = 630 word equiv.	up to 9 in.(228.6mm) high = 1260 word equiv.

D. Total Characters wide by Total Text lines = word equiv. as shown in the table above. **Add word equivalents** for each table in the column labeled **"Word Equivalents."**

Total Tables/Figures:	4887	(word equivalents)
Total Words of Text:	8289	

Total words and word equivalents:	**13176**
printed pages:	**11**

Estimating Length of Text

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Divided by 3	3	
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Count # of text lines per page	23	
# of words per page	291.33	
Count # of pages (don't add references & abstract)	19.5	
Title & Abstract	500	
Total # refs 63	1527	
Length of Text is	7708	subtototal
	581	plus headings
	8289	TOTAL words
	7	printed pages

Estimating Length of Tables & Figures:

Tables	Word Equivalents	**Figures**	Word Equivalents
Table 1	158	Figure 1	158
2	158	2	158
3	158	3	158
4	158	4	315
5	630	5	945
6	158	6	945
7	158	7	
8	630	8	
9		9	
10	0	10	
11	0	11	
12	0	12	
13	0	13	
14	0	14	
15	0	15	
Please double-up tables/figures if additional space is needed (ex. 20+21).		16	
		17	
		18	
		19	
		20 and 21	

updated 1/16/03