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Digital Twin for Next Gen Concretes: On-demand Tuning of Vulnerable Mixtures through Explainable and Anomalous Machine Learning

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Abstract

This paper presents a framework for integrating Explainable and Anomalous Machine Learning (EAML) into a digital twin to enable finetuning of mixtures as a mean to realize next-gen concretes with favorable performance. In this framework, both anomalous unsupervised and explainable supervised ML algorithms are joined to create a virtual assistant capable of exploring the influence of mixture materials and proportions on the required performance of concrete. This virtual assistant is not only trained to detect inherent vulnerabilities within mixtures but can also finetune such mixtures to overcome potential weaknesses – especially when concrete is expected to serve under extreme loading conditions. The proposed framework has been rigorously examined on three case studies to identify vulnerable mixtures to: 1) fire-induced spalling, 2) chloride penetration, and 3) failing to attain full design strength in job sites, using small and large datasets comprised from actual measurements. Results from our analysis show how the proposed framework was capable of identifying vulnerable concrete mixtures and of satisfying various performance metrics. While the proposed framework is designed to be algorithm-independent and hence can be scalable across multiple platforms, this work showcases the application of anomaly detecting and clustering algorithms, together with an ensemble of classifiers encompassing extreme and light gradient boosted trees (GBT), generalized additive models (GAM), and keras deep residual neural network (KDP).

Keywords: Machine learning; Digital twin; Concrete; Explainability; Clustering.

Introduction

The *digital twin* is often defined as the creation of a digitalized and comprehensive representation of a physical system, service, or product that includes valuable information gained throughout all of its lifecycle phases [1,2]. Once employed, a digital twin is expected to replicate the essence of the product on hand, thereby enabling real-time exploration and examination using data obtained from manufacturers, or feedbacks/experiences of users. Tracing the service history of a product is expected to provide us with valuable insights into the behavior and response of such a product – most of which are often missing during the research and development (R&D) stage. Once captured, such insights can prove elemental to significantly improve future generations of such a product [3]. Despite the success of this concept across various domains (i.e., manufacturing [4], robotics [5], etc.), the open literature seems to lack efforts on this front with regards to concrete as a construction material as opposed to modeling the construction phases of concrete structures [6].

A look into the use of concrete material reveals that concrete is used more than any other construction material globally, with a production rate reaching 10 billion tons (thus implying an average of 1.2 tons for each member of the world's population) [7]. This large production rate accounts for 5-8% of global carbon dioxide (CO2) emissions [8,9]. When dissected, the above infers two observations; 1) concrete is an attractive and wide-spread construction material and hence the amount of potential data available on concrete behavior is substantial, and 2) any improvements on this front will be valuable not only from a material performance point of view, but from an economic/environmental perspective as well [10,11]. This work argues that adopting a digital twin framework will enable us to realize improved concrete materials, which will translate to achieving sustainable and resilient concrete structures. This argument is built upon the notion that the behavior of structures is often governed by the response of its constituent materials to the surrounding environment [12,13].

Revisiting point no. 1 above shows that while we do have a large amount of data on concrete materials, such data is highly nonlinear and multi-dimensional [14]. Thus, a question arises as to how to efficiently collect and analyze such data? Herein where utilizing novel analytics tools becomes handy. For example, the use of machine learning (ML) has proven effective in handling high-dimensional and nonlinear datasets and hence can also be used to examine data on concrete materials [15,16]. In fact, the past few years have noted how ML techniques can be successfully applied to predict properties of concrete with high confidence. For example, Chopra et al. [17] compared compressive strength predictions from three algorithms (e.g., decision tree, random forest, and neural networks) and reported high accuracy exceeding 95%. In addition, Young et al. [18] analyzed over 10,000 concrete mix designs used in job sites as a means to arrive at insights between the mixture design variables and the 28-day compressive strength. These researchers reported adequate performance with an average relative error of less than 10% using neural networks.

In lieu of traditional ML, other works also applied advanced ML techniques. In one instance, Pazouki et al. [19] applied metaheuristics to estimate the compressive strength of self-compacting concretes. These researchers reported that metaheuristics produced higher prediction accuracy as compared to neural networks. Furthermore, a comprehensive examination was carried out by Chou et al. [20] to estimate the compressive strength of high-performance concrete on data collected from multiple nations. The main findings of Chou et al. [20] noted that ensemble learning techniques outperformed individual learning techniques in predicting strength property. In a parallel work, Yaseen et al. [21] applied extreme ML models (an improved version of neural networks) to evaluate the compressive strength of lightweight foamed concretes. Yaseen et al. [21] observed the merit and relatively high prediction capabilities of extreme ML techniques over traditional statistical methods. To a lesser degree, additional efforts also explored the use of advanced ML methods to examine the performance of concrete material under extreme conditions such as fire [22], and chloride penetration [23], among others [24–26].

Two primary observations can be drawn from the above reviewed works. The first observation notes that these works utilized ML algorithms that fall under supervised learning methods. Supervised learning comprises the majority of ML and is particularly applied in problems where both inputs and a target variable are labeled and known [27]. For instance, supervised learning can be applied when concrete mixture proportions are known and the strength associated with such mixture is also known. In this scenario, a ML algorithm can learn from the available data how to tie the inputs (e.g., mix proportions) to the target variable (i.e., strength property). This type of ML technique can be applied to two problem types; regression (when the target variable is a numeric value) and classification (when the target variable is a category, e.g., cracked/not cracked). The second observation notes that the above works, and by extension most works on property prediction of concrete, adopted Blackbox algorithms. Such algorithms have complex structures with inner workings that are intricate for a user to fathom. As such, users turn to be wary of such algorithms and may not trust their predictions – since they do not understand the justification behind model predictions. A move toward *explainable ML* where a model is capable of justifying its own predictions, is on the rise as it allows transparency and trust [28].

While supervised learning is commonly used in our domain, another type of learning is referred to as unsupervised learning, and this can be adopted in scenarios where only the inputs are available without any corresponding outputs. In this case, a ML algorithm is applied to explore the underlying structure within data to understand the nature of the problem on hand. Unsupervised learning can be broadly grouped into clustering (grouping by behavior, i.e., concrete mixtures of silicious nature tend to be more susceptible to fire-induced spalling than others [29]), association (discover rules that describe large portions of the assembled data, i.e., high strength concrete mixtures have a denser microstructure and hence could be vulnerable to spalling once heated), and anomaly detection (identifies observations that deviate from a dataset's normal behavior) [30]. At the time of this manuscript, the open literature only contains a few works that leverage unsupervised ML in the domain of concrete materials [31,32]. Exploring the full potential of unsupervised ML in this domain is another motivation behind this work.

In this pursuit, this paper aims to tie explainable and anomalous ML to realize a concrete digital twin that will allow users to finetune concrete mixture design on-demand, thereby negating issues during casting and deployment. This work is especially interested in identifying vulnerable mixtures to: 1) fire-induced spalling, 2) chloride penetration, and 3) irregularities in attaining design strength at job sites. To showcase the proposed framework, three case studies are undertaken using the following algorithms are used extreme and light gradient boosted trees (GBT), generalized additive models (GAM), and keras deep residual neural network (KDP), anomaly detecting, and k-means clustering algorithms. A complete examination of the performance of the proposed framework is provided in each case study.

Rationale to Integrating *EAML* into *Digital Twin*

This section covers the rationale for the proposed framework by adopting EAML into a digital twin from the lens of concrete materials.

Proposed framework

Figure 1 outlines a flowchart of the proposed framework. The proposed framework integrates two types of commonly used ML, unsupervised and supervised learning. This framework starts by examining a dataset on concrete mixtures via anomaly detection algorithms to identify and treat

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outliers. Outliers are anomalous observations that can be tied to a level of problem (or perhaps a measurement glitch), and hence such observations are to be correctly identified. Once such observations are identified, these can then be treated via a variety of means such as removal or substitution (e.g., with the average value of all observations, etc.), and can also be further analyzed to examine the inherent source of their outlierness (i.e., by examining equipment for re-calibration). One should also note that traditional statistical methods can be used to detect outliers [33]. However, recent works have noted the advantages of ML over such methods as they do not typically require numeric monotype attributes and can handle both multi-dimensional data and of symbolic attributes [34]. Given the stated motivation behind this work, we will be relying on ML for outlier detection in the examined three case studies[1].

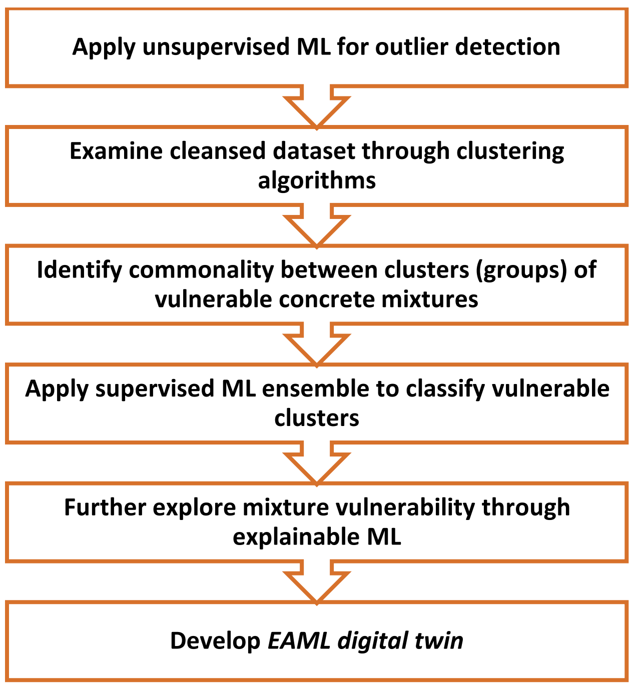

Fig. 1 Flowchart of the proposed framework

Once outliers are detected and treated, then the cleansed dataset is examined via a clustering algorithm. Clustering algorithms also fall under unsupervised learning and aim to cluster (or group) data of similar characteristics together. In theory, points that fall into one group would have similar properties that are unlike data in other groups. As such, a clustering analysis may enable users to gain valuable insights into how their data is clustered, as such clusters can be safely assumed to behave in a similar fashion [35]. The majority of clustering algorithms group data by

[1] For completion, the original references of case study no. 2 [23] and no. 3 [18] do provide a general discussion to outlier treatment through traditional statistical methods. Interested readers can refer to these works for such discussions.

examining how the data is spread or distant. As such, clustering can be undertaken via several methods, for example: centroid-based clustering, density-based clustering, and hierarchical clustering, etc. Commonly used clustering algorithms include k-means clustering, G-means clustering, Gaussian Mixture Models (GMMs), or Partitioning Around Medoids (PAM), etc. Given k-means' visual simplicity and wide use in literature [31,36], this work adopts the k-means algorithm to showcase the proposed framework (and the reader is reminded that other clustering algorithms can also be used).

At this stage, the dataset will be grouped into a number of independent clusters. As will be shown in the upcoming case studies, each cluster can be further examined not only to understand the commonality governing such cluster but to also relate such cluster to an expected mixture of concrete behavior (or performance). For instance, it is common for the large majority of proper mixtures (or those which have been shown to have an adequate performance) to be clustered together. Similarly, vulnerable mixtures can also be grouped into unique clusters, and these clusters can also be further investigated to arrive at the common mixture materials or proportions likely responsible for mixture vulnerability. Once such information is obtained, a user can then be trained to avoid using vulnerable mixtures.

Building on the above and noting how manually analyzing clusters in real-time is time-consuming and perhaps impractical, it is then thought of to leverage ML to assist users and concrete material designers. Hence, once vulnerable clusters are identified, a supervised ML classifier can be developed to classify if a given concrete mixture would fall under a "proper" mixture or a "vulnerable" mixture – thereby negating the need for constant human intervention and providing a practical solution that can be integrated/deployed into real scenarios. Furthermore, since most supervised ML models are Blackboxes (i.e., a user does not have the ability to understand why a given model generates a decision which is seen to restrict the use of ML in real scenarios [37]), our framework proposes to augment ML models with explainability tools to allow the user from understanding the reasoning behind the each of its decisions. For example, an explainable ML model can specify why a particular concrete mixture is classified as vulnerable by articulating the influence of which mixture ingredients have led to such classification (see Fig. 2). As one can see, having such a capability increases the level of trust between ML and concrete users.

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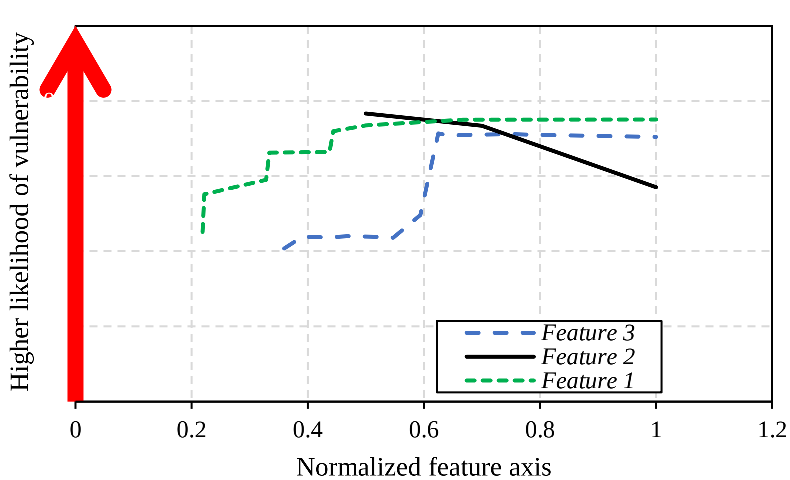

Figure 2 Illustration of explainability tool to identify responsible mixture features (i.e., ingredients) driving a ML model's decision

Recent works have noted how the reliance on a sole supervised ML classifier may yield to developing biased models or, in some instances, may not yield a near-optimal resolution effectively or timely [38,39]. As such, this work explores ensemble learning by means of multi-algorithmic search to achieve the most advantageous solution [40]. In this learning, a series of algorithms search together until a solution is identified. Then, a series of fitness metrics are applied to identify the fittest solution for a problem [41]. Following this procedure, the recognized solution is scrutinized across various search mechanisms and analysis stages.

Technical details and performance metrics

In all stages of ML analysis, each of the used algorithms is trained and validated on randomly shuffled sets of the dataset (which is being split into three sets, T: training, V: validation, and S: testing, in a 60%:20%:20% split). The algorithm is trained and validated on the T and V sets, respectively, using 10-fold cross-validation, and is then independently cross-checked by assessing the S (left-out) set that was not part of the training procedure. The 10-fold examination is also used to arrive at optimal hyper-tuning parameters for each model. Finally, performance metrics intended to measure the closeness of model prediction to that measured are applied [42–44].

In this work, three primary classification metrics are applied: the Area under the ROC curve (AUC) and Log Loss Error (LLE) – see Eqs. 1-2, as well as the confusion matrix [45–48]. The ROC curve is a graphical illustration that shows the performance of a classification ML model by plotting two parameters: true positive rate (TPR) and false positive rate (FPR). The second metric is referred to as the LLE, which yields a probability between zero and unity and penalizes for being too confident in the wrong prediction. The third metric that can be adopted to examine the performance of a classifier is known as the confusion matrix. Each row of this matrix represents the instances in the actual class, while each column represents the instances in the predicted class. Within this matrix, five supplementary metrics (including sensitivity, specificity, precision, negative predictive value, and accuracy) can also be evaluated, as noted in Eqs. 3-7.

$$AUC = \sum_{i=1}^{N-1} \frac{1}{2} (FP_{i+1} - FP_i)(TP_{i+1} - TP_i) \quad (1)$$

$$LLE = -\sum_{c=1}^{M} A_i log P \quad (2)$$

$$Sensitivity = \frac{TP}{P} = \frac{TP}{TP+FN} \quad (3)$$

Measures the proportion of actual positives that are correctly identified as positives.

$$Specificity = \frac{TN}{N} = \frac{TN}{TN+FP} \quad (4)$$

Measures the proportion of actual negatives that are correctly identified negatives.

$$Precision = \frac{TP}{TP+FP} \quad (5)$$

The proportions of positive observations that are true positives.

$$Negative\ Predictive\ Value\ (NPV) = \frac{TN}{TN+FN} \quad (6)$$

The proportions of negative observations that are true positives.

$$Accuracy = \frac{TP+TN}{P+N} = \frac{TP+TN}{TP+TN+FP+FN} \quad (7)$$

Evaluates the ratio of the number of correct predictions to the total number of samples.

where, P (denotes the number of real positives), N (denotes the number of real negatives), TP (denotes true positives), TN (denotes true negatives), FP (denotes false positives), and FN (denotes false negatives), M: number of classes, c: class label, y: binary indicator (0 or 1) if c is the correct classification for a given observation.

One should note that performance metrics are primarily available for supervised learning models since the dataset does include information on all variables, as well as the target of interest (i.e., "proper mixture" vs. "vulnerable mixture"). On the other hand, unsupervised ML models do not readily have performance metrics since the target of interest (i.e., number or types of clusters) is unknown beforehand. While the open literature does provide some insights and indexes that are tied to unsupervised ML models, these indexes can be applied to sample size and are primarily targeting the similarity of points within a cluster as opposed to the correctness of the number of clusters. For additional information on such metrics, the reader may refer to the Silhouette Coefficient [49] or Fowlkes-Mallows score [50]. The user is also reminded that the proposed framework can be augmented with such metrics if proven necessary.

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Selected Machine Learning Algorithms

This section describes the adopted algorithms in this work since their full description can be found elsewhere [51–55]. In all cases, the adopted algorithms were primarily applied in their default settings (unless otherwise specified) to create an ensemble that averages their predictions. The used algorithms can also be found at open-source and online repositories, as will be described henceforth. The proposed framework is algorithm-agnostic and hence is not only limited to the noted algorithms herein.

Anomaly detection algorithms

Two anomaly detection algorithms were used herein, namely, the isolation forest anomaly detection algorithm and the local outlier factor anomaly detection algorithm. The first algorithm isolates observations in a dataset by arbitrarily choosing a feature and then arbitrarily selecting a split value between the maximum and minimum values of the selected feature. This algorithm has a tree structure, and hence the number of splits required to isolate a sample is equivalent to the "path length" (which is a measure of normality where anomalies are linked to having shorter paths). This algorithm used 100 trees to start a random forest, with an expected outlier fraction of 10% as recommended by the developers of this algorithm which can be found herein [56,57]. The second algorithm measures the deviation of density of a particular observation with respect to its neighbors. Thus, by comparing the local density of an observation to the local densities of its neighbors, the algorithm can identify outliers as those with a substantially lower density than their neighbors. The applied algorithm can be found herein [58]. Both algorithms were combined into an ensemble that averages their predictions into normalized anomaly scores (with scores nearing unity implying higher anomalous behavior). An anomaly is considered when its anomaly score returns a value that is larger than 0.5 [56]. In lieu of the above algorithms, other anomaly algorithms can also be used, such as Mahalanobis distance [59].

k-means algorithm

The fundamental idea behind k-means clustering comprises of realizing a k number of center points (known as centroids) that minimize the total intra-cluster variation. Once the centers are realized, the points nearest to the same centroid are clustered together. Oftentimes, the k-means algorithm is applied iteratively to identify the optimal number of clusters in a dataset by examining the total decrease in intra-cluster variation attained from increasing the number of clusters. Once such variation is plotted for a series of clusters (e.g., k=2-10), then the optimal number of clusters can be visually identified as the point at which the curve bends (just like an elbow, and hence is commonly referred to as the elbow method [60]). This "elbow" point corresponds to the number of clusters to use. This algorithm leverages expectation maximization and aims at minimizing the squared error function. The adopted algorithm can be found at [61,62].

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Extreme Gradient Boosted Trees (ExGBT)

The ExGBT is a supervised serial model that combines predictions from weaker classifiers to optimize a differentiable loss function [63]. Briefly, the ExGBT algorithm matches predictions from successive trees to residual errors as a means to focus on complex cases to predict. This algorithm learns residual error directly rather than updating the weights of data points in other algorithms such as Random forest (RF). ExGBT can be found in [64,65]. ExGBT includes the following settings of learning rate of 0.01, "least squares regression loss" function, maximum tree depth of 8, subsample feature of 0.8, and 3000 for the number of boosting stages.

Light Gradient Boosted Trees (LGBT)

The LGBT is a light boosting algorithm that is relatively fast as it requires little processing time [66]. This algorithm shares similarities with the more commonly used RF algorithm. Unlike RF, the LGBT does not fit the trees in parallel; but rather, it fits the trees consecutively and then fits the residual errors from all the previous trees as well. The used algorithm can be found at [67] and was implemented with the following settings: learning rate = 0.1, maximum depth = "none", number of boosting stages = 500.

Generalized Additive Model (GAM)

The GAM is a simple algorithm that approximates nonlinear relationships via a linear formulation [68]of a series of smoothening functions. GAM can be represented by a linear formula or a table of coefficients. The adopted GAM incorporates a learning rate of 0.05, max depth of 3.0, with the number of boosting stages = 500.

Keras Deep Residual Neural Network (KDP)

KDP is a neural network model [69] with a direct connection linking data points to the target. This connection smoothens the loss function and enables network optimization. In the used KDP, a learning rate of 0.03 was used, along with a *Prelu* activation function, and two layers containing 512 neurons. KDP can be readily found at [70]. As mentioned earlier, an ensemble made of ExGBT, GAM, and KDP was created to average their predictions.

Case Studies

This section describes three case studies to be used in this work. These case studies will be examined via the proposed framework and steps that mirror those shown in Fig. 1. The three case studies aim to identify vulnerable concrete mixtures to fire-induced spalling, chloride penetration, and those that do not yield the design compressive strength at in-situ jobs.

Case study 1: Identifying mixtures vulnerable to fire-induced spalling

Fire-induced spalling is a complex phenomenon that occurs in concrete materials once exposed to fire conditions [71]. There has been an extensive body of works dedicated to investigating this phenomenon, many of which attributes its mechanisms to vapor pressure build-up, generation of thermal stresses, and the dense microstructure of high strength concrete, among others [72–75].

Despite the interest of this community in developing strategies to mitigate the adverse effects of fire-induced spalling, only a few works explored the use of traditional ML techniques in this area [76–78].

Herein, we aim to explore the influence of mixture ingredients on the propensity of spalling via EAML. Thus, in this case study, results from 169 fire tests on reinforced concrete columns are collected into a dataset [79]. This dataset contains information with regard to the occurrence of spalling, in addition to the concrete mixture used in each tested column and proportions. More specifically, the amount of cement, coarse and fine aggregate, aggregate type (carbonate, silicious, and lightweight), silica fume, fly ash, Polypropylene fibers, steel fibers, slag, and water is documented in kg/m^3 (see Fig. 3a). A Pearson correlation analysis of these components is also listed in Fig. 3b and 3c. It is clear that there is a strong correlation[2] between the characteristics of aggregates and cement with spalled columns.

The anomaly analysis starts by applying the anomaly ensemble to the dataset to, which noted the presence of six anomalous observations. These observations were then removed from the dataset. Then, the k-mean clustering analysis was initiated. This analysis noted the presence of four clusters (see Fig. 3d). As one can see, two clusters (clusters no. 1 and 4) reside on the left-hand side of this Biplot. A close examination of these clusters shows that they are highly related to the proportion of mixtures (with cluster no. 1 being tied to silica fume, fly ash, Polypropylene fibers, and steel fibers, and cluster no. 4 being tied to cement, coarse and fine aggregate, aggregate type and water). On the other hand, clusters no. 2 and 3 reside on the right-hand side of this figure, with cluster no. 2 being the farthest (implying a unique behavior within this cluster). Figure 3e further shows that mixtures in this cluster have significantly lesser values of cement, water, and coarse and fine aggregates. Hence, one can confidently say that cluster 2 is the most vulnerable of all mixtures as all columns within this cluster have spalled.

Thus, cluster no. 2 is labeled as "vulnerable", and the supervised ML ensemble is used to develop a virtual assistant to classify mixtures that may fall into this cluster as opposed to other clusters. This ensemble achieved the following metrics on training/validation/testing through AUC and LogLoss errors = 0.982/0.996/1.000, and 0.151/0.058/0.105, respectively. In addition, this ensemble also performed well under confusion matrix metrics (approaching unity), as noted in Fig. 3g. This matrix lists the number of observations that were correctly and wrongly predicted during the training/validation/testing of the models. For example, 114/22/28 implies that 114 specimens were used in the training and these were correctly predicted. In parallel, 22 and 28 specimens were examined during the validation and testing stages and these were also correctly tested, respectively.

[2] The reader must remember that this matrix shows the "linear" correlation between parameters. Other tools such as mutual information can be used to reveal association between parameters.

Hence, the developed tool can be used to identify concrete mixtures that are vulnerable to fire-induced spalling.

This tool can also pinpoint which components can lead to such vulnerability due to adopting explainability principles. Figure 3f illustrates the top five mixture ingredients that facilitate a mixture being of high likelihood to be in close proximity to those in cluster no. 2 (i.e., has a high vulnerability to spalling). These ingredients come to cement, water, and amount of coarse aggregate, aggregate type, and silica fume with 100%, 31%, 3%, 3%, and 1% impact on the classifier's decision (e.g., the classifier is highly sensitive to the amount of cement and water and these two ingredients are key features of mixtures in cluster no. 2). It can be seen that lower magnitudes of cement, water, and amount of coarse aggregate are linked to higher similarity to cluster no. 2, which implies a high propensity for spalling. Other ingredients, including aggregate type, silica fume, fly ash, etc., did not seem to contribute much to the classifier's decisions. Thus, mixtures deemed vulnerable to spalling can be automatically finetuned by manipulating the key parameters outlined in Fig. 3f to steer the mixture away from being very similar to those in cluster no. 2. For completion, Table 1 can be used to examine concrete mixtures and corresponding clusters manually.

Table 1 can be adopted for manual examination of concrete mixtures and their corresponding clusters to identify those vulnerable to spalling. A look into Table 1 shows that RC columns in all other clusters have suffered from spalling in some instances and also did not go under spalling. A further examination shows that only in cluster no. 2 that all specimens suffer from spalling, while specimens in other clusters spalled in some instances and did not undergo spalling in others. Special attention to cluster no. 4 reveals that 50% of all columns in this cluster have spalled, while the remaining 50% did not spall. As such, one can argue that cluster no. 4 can also be considered "vulnerable." If a user decides to go this route, then the developed ML classifier can be updated with such a decision to enable identifying concrete mixtures that may fall under cluster no. 2, or cluster no. 4. In this scenario, the classification problem changes from binary into a multi-class classification exercise which can be carried out with ease, as noted in earlier publications [41,80]. The problem may also maintain its binary nature by considering clusters no. 2 and 4 to be vulnerable if the user does not seek to uniquely pinpoint each vulnerable cluster independently.

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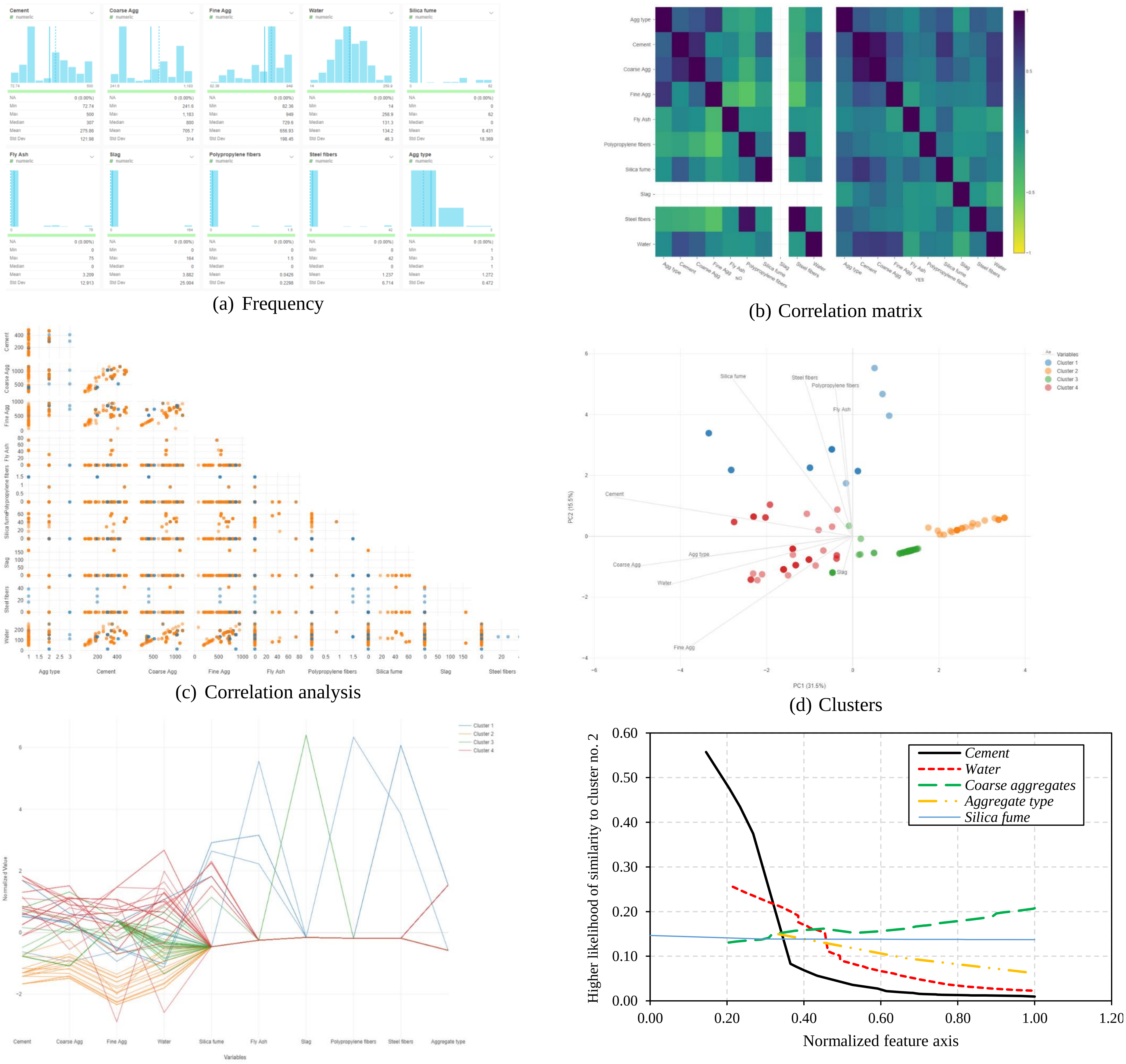

(a) Frequency

(b) Correlation matrix

(c) Correlation analysis

(d) Clusters

(e) Clusters per lines

(f) Impact of influencing ingredients

		Predicted True	Predicted False	Total
Actual	True	114/22/28	0/0/0	Sensitivity = 0.952
	False	1/1/0	20/4/6	Specifity = 1
		Precision = 1	NPV = 0.991	Accuracy = 0.993

(g) Confusion matrix (Training/Validation/Testing)

Fig. 3 Insights from EAML analysis

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Table 1 Further insights from clustering analysis on concrete mixtures

										cluster				
Spalling	Cement	Coarse Agg	Fine Agg	Water	Silica fume	Fly Ash	Slag	Polypropylene fibers	Steel fibers	1	2	3	4	Total
NO	158.19 - 243.64	241.60 - 429.88	429.02 - 602.34	111.95 - 160.93	0	0	0	1.5	17	1				1
									27	1				1
									39	1				1
			602.34 - 775.67	62.98 - 111.95	0	0	0	0	0			4		4
				111.95 - 160.93	0	0	0	0	0			10		10
	243.64 - 329.10	994.72 - 1,183.00	775.67 - 949.00	14.00 - 62.98	0	0	0	0	0				2	2
				111.95 - 160.93	0	0	0	0	0				21	21
	329.10 - 414.55	618.16 - 806.44	775.67 - 949.00	209.90 - 258.88	0	0	0	0	0				2	2
		806.44 - 994.72	429.02 - 602.34	111.95 - 160.93	0	75	0	0	0	1				1
		994.72 - 1,183.00	775.67 - 949.00	160.93 - 209.90	0	0	0	0	0				4	4
	414.55 - 500.00	429.88 - 618.16	602.34 - 775.67	111.95 - 160.93	0	0	0	0	0				2	2
		806.44 - 994.72	602.34 - 775.67	160.93 - 209.90	42	0	0	0.9	0	1				1
		994.72 - 1,183.00	429.02 - 602.34	160.93 - 209.90	0	0	0	0	0				4	4
			602.34 - 775.67	160.93 - 209.90	42	0	0	0	0				1	1
YES	72.74 - 158.19	241.60 - 429.88	82.36 - 255.69	14.00 - 62.98	0	0	0	0	0		7			7
				62.98 - 111.95	0	0	0	0	0		1			1
			255.69 - 429.02	62.98 - 111.95	0	0	0	0	0		13			13
		429.88 - 618.16	255.69 - 429.02	62.98 - 111.95	0	0	0	0	0		4			4
	158.19 - 243.64	241.60 - 429.88	602.34 - 775.67	62.98 - 111.95	0	0	0	0	0			12		12
				111.95 - 160.93	0	0	0	0	0			17		17
		429.88 - 618.16	255.69 - 429.02	62.98 - 111.95	0	0	0	0	0		1			1
		618.16 - 806.44	255.69 - 429.02	111.95 - 160.93	0	0	0	0	0		1			1
			602.34 - 775.67	160.93 - 209.90	0	0	0	0	0			4		4
	243.64 - 329.10	618.16 - 806.44	602.34 - 775.67	111.95 - 160.93	29.5	0	0	0	0			1	1	2
		806.44 - 994.72	602.34 - 775.67	160.93 - 209.90	0	0	0	0	0				2	2
				209.90 - 258.88	0	0	0	0	0				1	1
		994.72 - 1,183.00	775.67 - 949.00	111.95 - 160.93	0	0	0	0	0				1	1
				209.90 - 258.88	0	0	0	0	0				2	2
	329.10 - 414.55	618.16 - 806.44	429.02 - 602.34	62.98 - 111.95	57	32	0	0	0	3				3
					62	44	0	0	0	4				4
			775.67 - 949.00	209.90 - 258.88	0	0	0	0	0				1	1
		806.44 - 994.72	429.02 - 602.34	111.95 - 160.93	0	0	0	0	0			1		1
						75	0	0	0	2				2
					18.2	45.4	0	0	0	1				1
					36.3	0	0	0	0				2	2
			775.67 - 949.00	160.93 - 209.90	0	0	0	0	0				7	7
		994.72 - 1,183.00	82.36 - 255.69	209.90 - 258.88	0	0	0	0	0				1	1
			602.34 - 775.67	62.98 - 111.95	0	0	164	0	0			4		4
			775.67 - 949.00	160.93 - 209.90	0	0	0	0	0				1	1
	414.55 - 500.00	806.44 - 994.72	602.34 - 775.67	160.93 - 209.90	42	0	0	0	42	3				3
								0.9	0	2				2
			775.67 - 949.00	160.93 - 209.90	50	0	0	0	0				5	5
		994.72 - 1,183.00	429.02 - 602.34	160.93 - 209.90	0	0	0	0	0				2	2
			602.34 - 775.67	111.95 - 160.93	51	0	0	0	0				2	2
				160.93 - 209.90	42	0	0	0	0				5	5
Total										20	27	53	69	169

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Case study 2: Identifying mixtures vulnerable to chloride penetration

Chloride ions generated by marine or coastal environments can accumulate or leech on concrete structures and penetrate the underlying layers of concrete. Once successfully penetrate the deep layers of concrete, chloride ions can accelerate corrosion of steel reinforcement which may eventually lead to concrete cracking [23]. Thus, mitigating chloride penetration becomes of utmost importance to satisfy durability requirements set forth by building codes (such as ACI 318 [81]). In general, four classes describe chloride exposure: atmospheric, tidal, splash, and submerged. This case study focuses on tidal exposure and uses 386 field measurements recently collected by Cai et al. [23].

In their work, Cai et al. [23] applied traditional regression ML models to predict surface chloride concentration (C_s) of concrete and reported adequate performance of coefficient of determination (R^2) ranging from 0.46 to 0.83. In this case study, we will apply EAML to classify concrete mixtures that have a high vulnerability to attaining a high concentration of C_s. As mentioned earlier, the collected 386 observations contained complete information with regard to concrete mixture designs, environmental conditions, and exposure time (see Fig. 4a). More specifically, this information includes proportions of ordinary Portland cement (*OPC*), fly ash (*FA*), ground-granulated blast-furnace slag (*GGBS*), silica fume (*SF*), superplasticizer, water, fine aggregate, and coarse aggregate (in kg/m^3), characteristics of environmental conditions (annual mean temperature (°C), and chloride concentration (*Cl*) in seawater (in g/L)), and exposure time (units of annual)) [23]. Figures 4b and 4c show a glimpse of the outcome of Pearson correlation analysis of all parameters included in the aforenoted dataset. One can see a strong linear correlation between fine aggregates, silica fume, superplasticizers with chloride concentration.

Similar to the analysis carried out in the first case study, the anomaly investigation was undertaken first. This investigation noted the presence of ten anomalous observations, which were removed from the dataset. The anomaly analysis was followed by the clustering analysis. Results from the k-means clustering are shown in Fig. 4d and demonstrate the existence of five clusters. At first glance, cluster no. 1 is the farthest from the center of the Biplpot chart compared to other clusters. On the other hand, clusters no. 2 and no. 3 are governed by the amount of *GGBs* and exposure time and coarse aggregates (with cluster no. 3 being more reliant on coarse aggregates than cluster no. 2). Finally, cluster no. 4 is primarily governed by the amount of *OPC*, *SF*, *Cl*, Fine aggregates, and superplasticizers, while cluster no. 5 is solely governed by *FA*. To complement the k-means analysis, a look into Fig. 4e shows how among all clusters, clusters no. 1 and no. 2 seem to have the most significant disturbance near the examined variables.

Table 2 can be used for manual examination of concrete mixtures and corresponding clusters. It is quite clear that clusters no. 1 and no. 2 only underwent low concentrations of chloride when compared to all other clusters. This implies that mixtures in other clusters 3, 4 and 5 can be vulnerable to chloride penetration much more than those in clusters no. 1 and no. 2. Hence, clusters no. 3, 4, and 5 are labeled as "vulnerable" and users/engineers are asked to consider the chloride-based vulnerability of adopting mixtures from such clusters.

Upon training and cross-validation, the developed ensemble achieved the following high ranking metrics on training/validation/testing through AUC and LogLoss errors = 1.000/1.000/1.000, and 0.053/0.045/0.042, respectively. Other metrics related to the confusion matrix also performed well (approaching unity), as noted in Fig. 4g. This matrix lists the number of observations that were correctly and wrongly predicted during the training/validation/testing of the models. For example, 42/9/11 means that 42 specimens were used in the training and were correctly predicted. Similarly, 9 and 11 specimens were used in the validation and testing of the models and were also correctly tested, respectively. Finally, a similar approach can be used to describe 265/53/66.

By adopting explainability principles, Fig. 4f can be used to identify the top five critical mixture components that can be linked to a concrete mixture being of high likelihood to be in close proximity to those in clusters no. 3, 4, or 5 (i.e., has a high vulnerability to chloride penetration). These ingredients come from water, coarse aggregate, exposure time, superplasticizers, and *OPC* with 100%, 94%, 91%, 89%, and 52% impact on the classifier's decision. Figure 4f shows that mixtures with high quantities of water, coarse aggregates, and *OPC* are highly linked to having a high propensity to chloride penetration.

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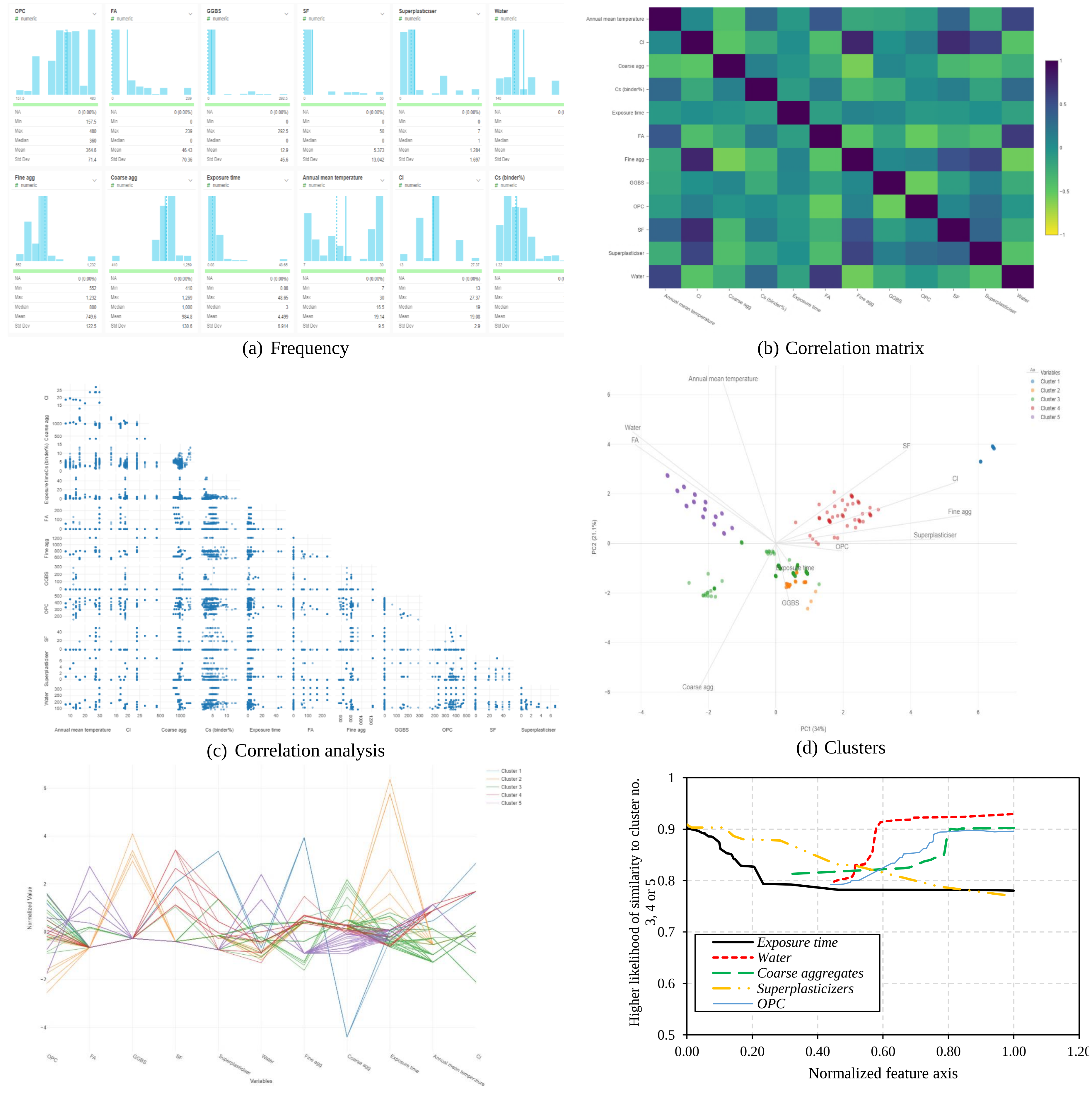

(a) Frequency (b) Correlation matrix

(c) Correlation analysis (d) Clusters

(e) Clusters per lines (f) Impact of influencing ingredients

		Predicted: True	Predicted: False	Total
Actual	True	42/9/11	1/0/0	Sensitivity = 1
	False	1/0/0	265/53/66	Specifity = 1
		Precision = 1	NPV = 1	Accuracy = 1

(g) Confusion matri (Training/Validation/Testing)

Fig. 4 Insights from EAML analysis

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Table 2 Further insights from clustering analysis on concrete mixtures

Cs (binder%)	OPC	Coarse agg	Fine agg	FA	Water	CI	Exposure time	Annual mean temperature	GGBS	cluster 1	2	3	4	5	Total
1.32 - 5.41	157.50 - 222.00	925.40 - 1,097.20	688.00 - 824.00	0	140.00 - 174.20	19	0.08 - 9.79	14	148		4				4
									200		4				4
	222.00 - 286.50	753.60 - 925.40	552.00 - 688.00	239	242.60 - 276.80	17	0.08 - 9.79	30	0					3	3
					276.80 - 311.00	17	0.08 - 9.79	30	0					4	4
		925.40 - 1,097.20	552.00 - 688.00	239	208.40 - 242.60	17	0.08 - 9.79	30	0					7	7
			688.00 - 824.00	0	140.00 - 174.20	19	0.08 - 9.79	14	165		4				4
					174.20 - 208.40	19	9.79 - 19.51	14	160		4				4
									168		6				6
				80	140.00 - 174.20	19	0.08 - 9.79	12.3	140		4				4
	286.50 - 351.00	753.60 - 925.40	552.00 - 688.00	167	242.60 - 276.80	17	0.08 - 9.79	30	0					5	5
					276.80 - 311.00	17	0.08 - 9.79	30	0					4	4
		925.40 - 1,097.20	552.00 - 688.00	167	208.40 - 242.60	17	0.08 - 9.79	30	0					7	7
			688.00 - 824.00	0	140.00 - 174.20	19	0.08 - 9.79	12.3	135		1				1
							19.51 - 29.22	14	0		4				4
							38.94 - 48.65	14	0		3				3
					174.20 - 208.40	23.96	0.08 - 9.79	27.5	0				8		8
								30	0				1		1
				60	174.20 - 208.40	19	0.08 - 9.79	7	0			43			43
				135	140.00 - 174.20	19	0.08 - 9.79	12.3	0			1			1
			824.00 - 960.00	0	140.00 - 174.20	23.96	0.08 - 9.79	30	0				1		1
		1,097.20 - 1,269.00	688.00 - 824.00	0	140.00 - 174.20	18.5	0.08 - 9.79	16.8	0			8			8
	351.00 - 415.50	753.60 - 925.40	552.00 - 688.00	72	276.80 - 311.00	17	0.08 - 9.79	30	0					2	2
				119	276.80 - 311.00	17	0.08 - 9.79	30	0					3	3
		925.40 - 1,097.20	552.00 - 688.00	72	208.40 - 242.60	17	0.08 - 9.79	30	0					3	3
					242.60 - 276.80	17	0.08 - 9.79	30	0					4	4
				119	208.40 - 242.60	17	0.08 - 9.79	30	0					4	4
					242.60 - 276.80	17	0.08 - 9.79	30	0					4	4
			688.00 - 824.00	0	140.00 - 174.20	19	0.08 - 9.79	12.3	67.5			1			1
								14	0			5			5
							38.94 - 48.65	14	0		5				5
						23.96	0.08 - 9.79	27	0				2		2
					174.20 - 208.40	19	0.08 - 9.79	7	0			35			35
						23.96	0.08 - 9.79	27.5	0				7		7
								30	0				2		2
					208.40 - 242.60	16.5	0.08 - 9.79	20.2	0			2			2
							9.79 - 19.51	20.2	0			1			1
				67.5	140.00 - 174.20	19	0.08 - 9.79	12.3	0			1			1
			824.00 - 960.00	0	140.00 - 174.20	23.96	0.08 - 9.79	27	0				3		3
								27.5	0				4		4
								30	0				2		2
	415.50 - 480.00	410.00 - 581.80	1,096.00 - 1,232.00	0	140.00 - 174.20	23.96	0.08 - 9.79	23.5	0	4					4
						27.37	0.08 - 9.79	27.5	0	9					9
		753.60 - 925.40	552.00 - 688.00	0	276.80 - 311.00	17	0.08 - 9.79	30	0					2	2
		925.40 - 1,097.20	552.00 - 688.00	0	208.40 - 242.60	17	0.08 - 9.79	30	0			2			2
					242.60 - 276.80	17	0.08 - 9.79	30	0					3	3
			688.00 - 824.00	0	140.00 - 174.20	19	0.08 - 9.79	14	0			5			5
					174.20 - 208.40	19.8	0.08 - 9.79	10	0			26			26
					208.40 - 242.60	16.5	0.08 - 9.79	20.2	0			4			4
							9.79 - 19.51	20.2	0			2			2
		1,097.20 - 1,269.00	552.00 - 688.00	0	174.20 - 208.40	13	0.08 - 9.79	16.5	0			3			3
5.41 - 9.49	157.50 - 222.00	925.40 - 1,097.20	688.00 - 824.00	0	140.00 - 174.20	19	0.08 - 9.79	12.3	292.5		1				1
	222.00 - 286.50	753.60 - 925.40	552.00 - 688.00	239	242.60 - 276.80	17	0.08 - 9.79	30	0					5	5
					276.80 - 311.00	17	0.08 - 9.79	30	0					4	4
		925.40 - 1,097.20	552.00 - 688.00	239	208.40 - 242.60	17	0.08 - 9.79	30	0					1	1
			688.00 - 824.00	0	140.00 - 174.20	19	0.08 - 9.79	12.3	225		1				1
	286.50 - 351.00	753.60 - 925.40	552.00 - 688.00	167	242.60 - 276.80	17	0.08 - 9.79	30	0					3	3
					276.80 - 311.00	17	0.08 - 9.79	30	0					4	4
		925.40 - 1,097.20	552.00 - 688.00	167	208.40 - 242.60	17	0.08 - 9.79	30	0					1	1
			688.00 - 824.00	0	174.20 - 208.40	23.96	0.08 - 9.79	27.5	0				2		2
				60	174.20 - 208.40	19	0.08 - 9.79	7	0			6			6
			824.00 - 960.00	0	140.00 - 174.20	23.96	0.08 - 9.79	27.5	0				2		2
	351.00 - 415.50	753.60 - 925.40	552.00 - 688.00	72	276.80 - 311.00	17	0.08 - 9.79	30	0					6	6
				119	276.80 - 311.00	17	0.08 - 9.79	30	0					5	5
		925.40 - 1,097.20	552.00 - 688.00	72	208.40 - 242.60	17	0.08 - 9.79	30	0					5	5
					242.60 - 276.80	17	0.08 - 9.79	30	0					4	4
				119	208.40 - 242.60	17	0.08 - 9.79	30	0					4	4
					242.60 - 276.80	17	0.08 - 9.79	30	0					4	4
			688.00 - 824.00	0	174.20 - 208.40	23.96	0.08 - 9.79	27.5	0				9		9
			824.00 - 960.00	0	140.00 - 174.20	23.96	0.08 - 9.79	27.5	0				7		7
		1,097.20 - 1,269.00	552.00 - 688.00	0	174.20 - 208.40	13	0.08 - 9.79	16.5	0			1			1
	415.50 - 480.00	753.60 - 925.40	552.00 - 688.00	0	276.80 - 311.00	17	0.08 - 9.79	30	0					2	2
		925.40 - 1,097.20	552.00 - 688.00	0	208.40 - 242.60	17	0.08 - 9.79	30	0			2			2
					242.60 - 276.80	17	0.08 - 9.79	30	0					1	1
			688.00 - 824.00	0	174.20 - 208.40	19.8	0.08 - 9.79	10	0			11			11
		1,097.20 - 1,269.00	552.00 - 688.00	0	174.20 - 208.40	13	0.08 - 9.79	16.5	0			6			6
9.49 - 13.58	286.50 - 351.00	1,097.20 - 1,269.00	552.00 - 688.00	0	174.20 - 208.40	13	0.08 - 9.79	16.5	0			4			4
				57	174.20 - 208.40	13	0.08 - 9.79	16.5	0					1	1
				76	174.20 - 208.40	13	0.08 - 9.79	16.5	0					1	1
	351.00 - 415.50	925.40 - 1,097.20	688.00 - 824.00	0	174.20 - 208.40	23.96	0.08 - 9.79	27.5	0				2		2
			824.00 - 960.00	0	140.00 - 174.20	23.96	0.08 - 9.79	27.5	0				1		1
		1,097.20 - 1,269.00	552.00 - 688.00	0	174.20 - 208.40	13	0.08 - 9.79	16.5	0			3			3
	415.50 - 480.00	925.40 - 1,097.20	688.00 - 824.00	0	174.20 - 208.40	19.8	0.08 - 9.79	10	0			1			1
Total										13	41	173	53	106	386

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Case study 3: Identifying mixtures vulnerable to failing to develop full design strength at in-situ conditions

In a recent study, Young et al. [18,82] present a large dataset encompassing 10,000 concrete mixtures and their corresponding measured compressive strengths from in-situ (job-site) as provided by an international vertically-integrated cement/concrete producer (VIP). This dataset was built by averaging measured compressive strength attained from testing three standard concrete cylinders that were cured following ASTM C39 for 28 days. The data set contained mixture proportions in terms of water, cement, and fly ash contents (in kg/m^3 of concrete), water-reducing admixture (*WRA*) and air-entraining admixture contents (*AEA* in 0.01kg/ kg of cementitious material), coarse and fine aggregate contents (in kg/m^3 of concrete), and fresh air content (in volume %), and measured compressive strength for each mixture. This study then explores the use of regression-based ML algorithms to develop a model capable of predicting the 28-day compressive strength of concrete. These researchers reported achieving good prediction metrics ranging between 0.49-0.59 in terms of R^2 and 9-10% in terms of mean absolute percentage error (*MAPE*). The same researchers point out challenges that arose during their work which can be summed by the fact that complied dataset spans a considerable timeframe and includes diversity in: ambient weather conditions, quality, and composition of raws, as well as mixing procedure.

Mimicking the previous two case studies, our analysis starts by removing outliers through the anomaly detection algorithms. Then, the cleansed dataset is examined via the k-means clustering algorithm to reveal four unique clusters (see Biplot in Fig. 5d). As one can see, cluster no. 3 resides on the right-hand side of this plot and seems to be influenced by *AEA* and *WRA* doses. On the other hand, clusters no. 1, and 2 are centralized near the center of the Biplot. Cluster no. 1 is governed by fine aggregates and water to binder ratio, while cluster no. 2 is mainly influenced by fly ash, *AEA* dose, and strength. Both clusters no. 1 and no. 2 are slightly influenced by aggregate amount.

Figure 5e lays out how each cluster is influenced by all mixture proportions combined. It is noteworthy to mention that of all clusters, mixtures belonging to cluster no. 3 performed on the lower side of this figure (i.e., have lower amounts than the average or normalized mean in coarse and fine aggregates, weight, and fly ash). A cross-examination of Table 3 reveals that the number of mixtures that did not develop their intended compressive design strength as compared to the total number of samples in each cluster is 53/2772 = 1.9%, 163/5538 = 2.9%, and 53/1320 = 4% for clusters no. 1, 2 and 3, respectively. This shows that mixtures belonging to cluster no. 3 seem to be the most vulnerable – which also agrees with observations of Fig. 5e.

At this point, the supervised and explainable ML ensemble is trained to classify mixtures belonging to cluster no. 3 as "vulnerable". The ensemble achieved the following metrics in training/validation/testing through AUC and LogLoss errors = 0.999/0.998/1.000, and 0.012/0.017/0.007, respectively. These metrics, together with those relating to the confusion matrix listed in Fig. 5g, show the high predictive capability of this ensemble classifier – a similar description of the results of this matrix can mirror that in the previous two case studies. Figure 5f points out the impact of the top five influencing factors driving the rationale of the ensemble as coarse aggregates (100%), weight (80%), fine aggregates (28%), fly ash (9%), and water-binder ratio (7%) by using the explainability principles. This figure shows that having lower amounts of the above parameters may lead to a mixture being similar to those attached to cluster no. 3.

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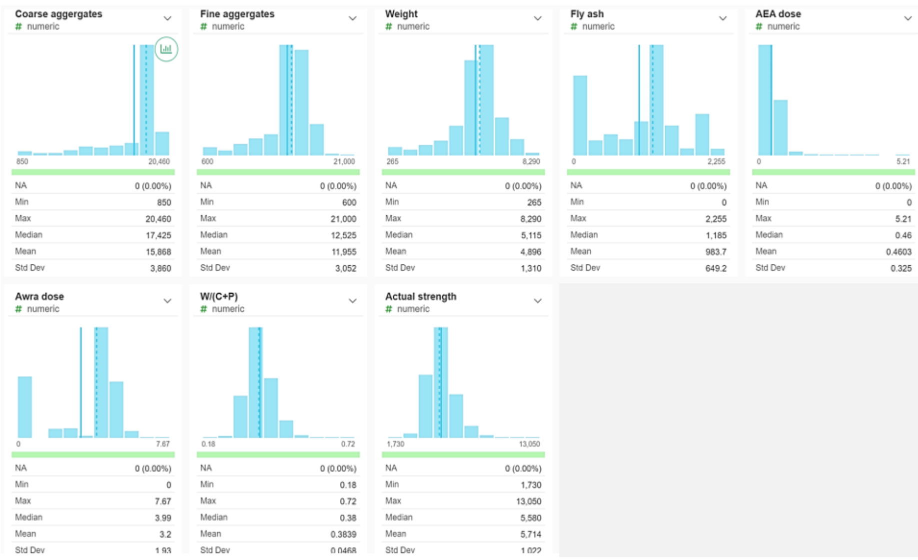
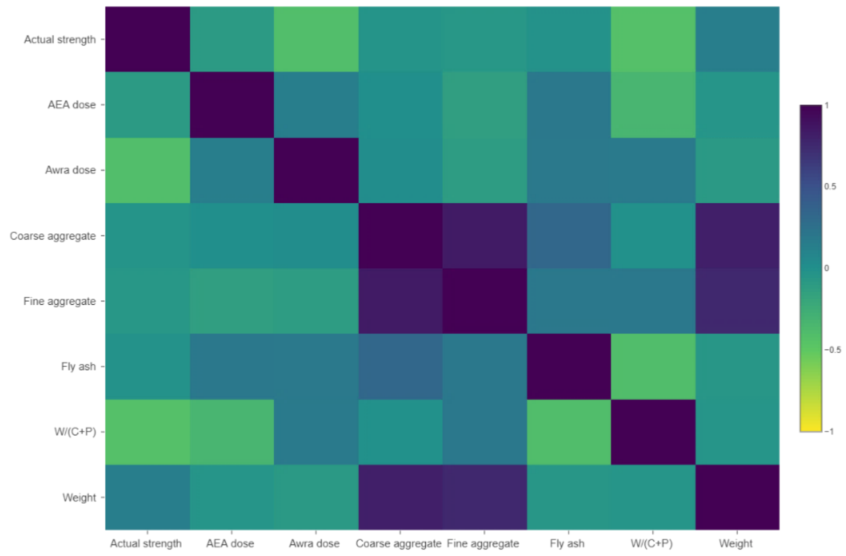
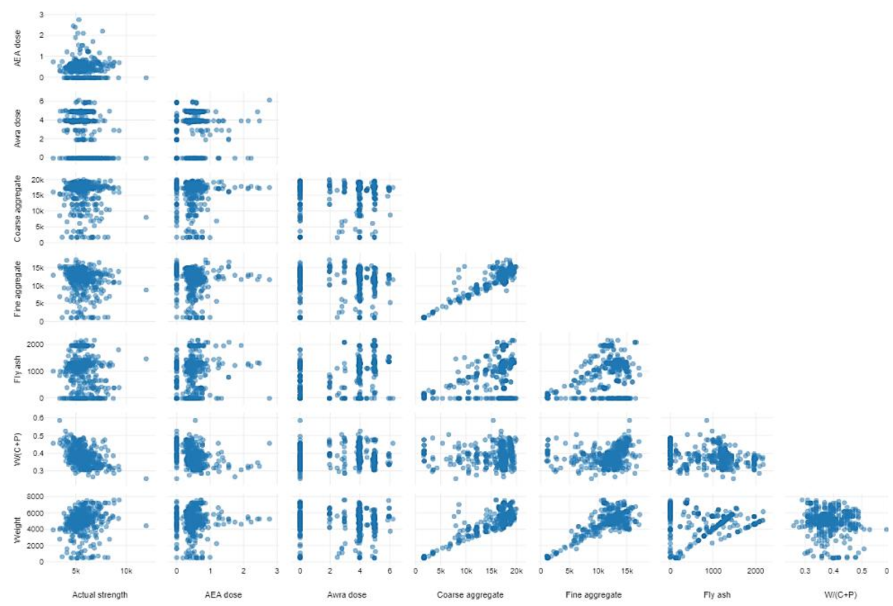


(a) Frequency

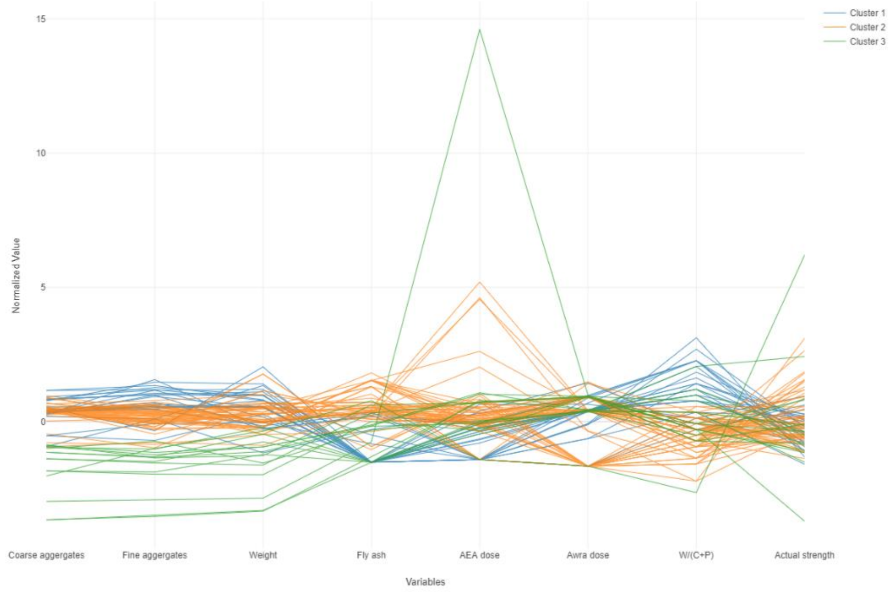


(b) Correlation matrix

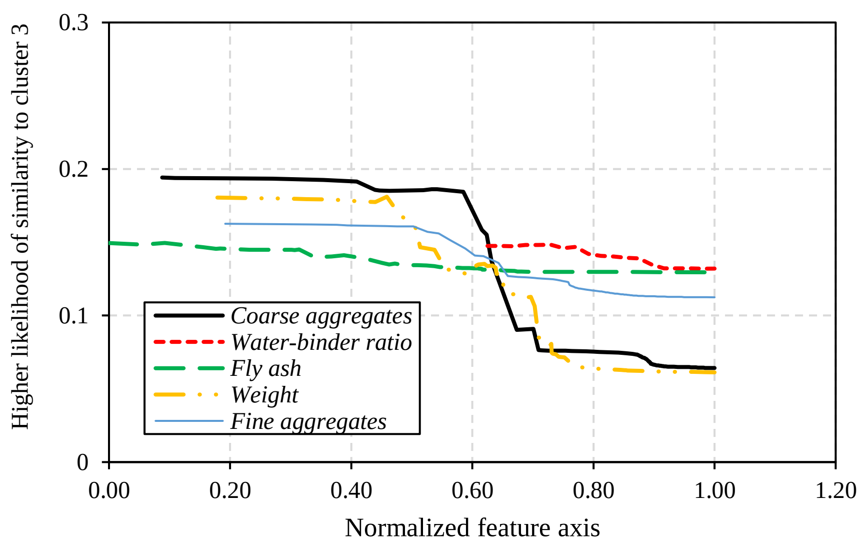


(c) Correlation analysis

(d) Clusters



(e) Clusters per lines



(f) Impact of influencing ingredients

		Predicted: True	Predicted: False	Total
Actual	True	1550/308/391	19/6/1	Sensitivity = 0.994
	False	40/3/9	6137/1233/1536	Specifity = 0.997
		Precision = 0.999	NPV = 0.978	Accuracy = 0.995

(g) Confusion matrix (Training/Validation/Testing)

Fig. 5 Insights from EAML analysis

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Table 3 Further insights from clustering analysis on concrete mixtures

							cluster			
Poor strength	Actual strength	Coarse aggergates	Fine aggergates	W/(C+P)	Weight	AEA dose	1	2	3	Total
no	1,730.00 - 5,503.33	850.00 - 7,386.67	600.00 - 7,400.00	0.18 - 0.36	265.00 - 1,870.00	0.00 - 1.04			48	48
						1.04 - 2.08			1	1
						2.08 - 3.13			1	1
					1,870.00 - 3,475.00	0.00 - 1.04			13	13
				0.36 - 0.54	265.00 - 1,870.00	0.00 - 1.04			118	118
						1.04 - 2.08			2	2
					1,870.00 - 3,475.00	0.00 - 1.04			23	23
						1.04 - 2.08			1	1
				0.54 - 0.72	265.00 - 1,870.00	0.00 - 1.04			2	2
			7,400.00 - 14,200.00	0.18 - 0.36	1,870.00 - 3,475.00	0.00 - 1.04			1	1
					5,080.00 - 6,685.00	0.00 - 1.04		1		1
				0.36 - 0.54	1,870.00 - 3,475.00	0.00 - 1.04			4	4
		7,386.67 - 13,923.33	600.00 - 7,400.00	0.18 - 0.36	1,870.00 - 3,475.00	0.00 - 1.04			51	51
					3,475.00 - 5,080.00	0.00 - 1.04			2	2
				0.36 - 0.54	265.00 - 1,870.00	0.00 - 1.04			1	1
					1,870.00 - 3,475.00	0.00 - 1.04			92	92
					3,475.00 - 5,080.00	0.00 - 1.04			8	8
			7,400.00 - 14,200.00	0.18 - 0.36	1,870.00 - 3,475.00	0.00 - 1.04		1	28	29
					3,475.00 - 5,080.00	0.00 - 1.04		15	14	29
						1.04 - 2.08		2		2
					5,080.00 - 6,685.00	0.00 - 1.04	2		2	4
					6,685.00 - 8,290.00	0.00 - 1.04	2			2
				0.36 - 0.54	1,870.00 - 3,475.00	0.00 - 1.04	13	3	86	102
					3,475.00 - 5,080.00	0.00 - 1.04	40	33	58	131
						1.04 - 2.08		1		1
					5,080.00 - 6,685.00	0.00 - 1.04	11	4		15
					6,685.00 - 8,290.00	0.00 - 1.04	1			1
				0.54 - 0.72	1,870.00 - 3,475.00	0.00 - 1.04	1			1
				0.54 - 0.72	1,870.00 - 3,475.00	0.00 - 1.04	1			1
			14,200.00 - 21,000.00	0.36 - 0.54	3,475.00 - 5,080.00	0.00 - 1.04	22			22
					5,080.00 - 6,685.00	0.00 - 1.04	12			12
						1.04 - 2.08		1		1
					6,685.00 - 8,290.00	0.00 - 1.04	1			1
		13,923.33 - 20,460.00	7,400.00 - 14,200.00	0.18 - 0.36	3,475.00 - 5,080.00	0.00 - 1.04		385		385
						1.04 - 2.08		23		23
						2.08 - 3.13		2		2
					5,080.00 - 6,685.00	0.00 - 1.04	6	273		279
						1.04 - 2.08		31		31
						2.08 - 3.13		5		5
					6,685.00 - 8,290.00	0.00 - 1.04	5			5
				0.36 - 0.54	1,870.00 - 3,475.00	0.00 - 1.04	2	3		5
					3,475.00 - 5,080.00	0.00 - 1.04	150	660		810
						1.04 - 2.08		3		3
						2.08 - 3.13		1		1
					5,080.00 - 6,685.00	0.00 - 1.04	418	635		1,053
						1.04 - 2.08	3	7		10
						2.08 - 3.13		1		1
					6,685.00 - 8,290.00	0.00 - 1.04	41			41
			14,200.00 - 21,000.00	0.18 - 0.36	3,475.00 - 5,080.00	0.00 - 1.04		22		22
						1.04 - 2.08		12		12
					5,080.00 - 6,685.00	0.00 - 1.04	2	22		24
						1.04 - 2.08		14		14
				0.36 - 0.54	3,475.00 - 5,080.00	0.00 - 1.04	285	56		341
						1.04 - 2.08		10		10
					5,080.00 - 6,685.00	0.00 - 1.04	354	61		415
						1.04 - 2.08	6			6
					6,685.00 - 8,290.00	0.00 - 1.04	29			29
				0.54 - 0.72	1,870.00 - 3,475.00	0.00 - 1.04	2			2
					3,475.00 - 5,080.00	0.00 - 1.04	8			8
	5,503.33 - 9,276.67	850.00 - 7,386.67	600.00 - 7,400.00	0.18 - 0.36	265.00 - 1,870.00	0.00 - 1.04			78	78
					1,870.00 - 3,475.00	0.00 - 1.04			35	35
						1.04 - 2.08			2	2
				0.36 - 0.54	265.00 - 1,870.00	0.00 - 1.04			129	129
						1.04 - 2.08			2	2
					1,870.00 - 3,475.00	0.00 - 1.04			23	23
				0.54 - 0.72	265.00 - 1,870.00	0.00 - 1.04			1	1
			7,400.00 - 14,200.00	0.18 - 0.36	3,475.00 - 5,080.00	0.00 - 1.04			2	2
					5,080.00 - 6,685.00	0.00 - 1.04		2		2
				0.36 - 0.54	1,870.00 - 3,475.00	0.00 - 1.04			2	2
					3,475.00 - 5,080.00	0.00 - 1.04	1		4	5
					5,080.00 - 6,685.00	0.00 - 1.04		4		4
			14,200.00 - 21,000.00	0.18 - 0.36	5,080.00 - 6,685.00	0.00 - 1.04		1		1
				0.36 - 0.54	5,080.00 - 6,685.00	0.00 - 1.04	1	1		2
					6,685.00 - 8,290.00	0.00 - 1.04	1			1
		7,386.67 - 13,923.33	600.00 - 7,400.00	0.18 - 0.36	1,870.00 - 3,475.00	0.00 - 1.04			97	97
						1.04 - 2.08			1	1
					3,475.00 - 5,080.00	0.00 - 1.04		1	19	20
						1.04 - 2.08			1	1
				0.36 - 0.54	1,870.00 - 3,475.00	0.00 - 1.04			91	91
					3,475.00 - 5,080.00	0.00 - 1.04			23	23
			7,400.00 - 14,200.00	0.18 - 0.36	1,870.00 - 3,475.00	0.00 - 1.04		4	42	46
					3,475.00 - 5,080.00	0.00 - 1.04	5	52	46	103
					5,080.00 - 6,685.00	0.00 - 1.04	1	9	3	13
					6,685.00 - 8,290.00	0.00 - 1.04	2			2

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							cluster			
Poor strength	Actual strength	Coarse aggergates	Fine aggergates	W/(C+P)	Weight	AEA dose	1	2	3	Total
				0.36 - 0.54	1,870.00 - 3,475.00	0.00 - 1.04	2	3	70	75
					3,475.00 - 5,080.00	0.00 - 1.04	79	35	78	192
					5,080.00 - 6,685.00	0.00 - 1.04	12	2		14
					6,685.00 - 8,290.00	0.00 - 1.04	1			1
			14,200.00 - 21,000.00	0.18 - 0.36	6,685.00 - 8,290.00	0.00 - 1.04	2			2
				0.36 - 0.54	3,475.00 - 5,080.00	0.00 - 1.04		1		1
					5,080.00 - 6,685.00	0.00 - 1.04	36	3		39
					6,685.00 - 8,290.00	0.00 - 1.04	3			3
				0.54 - 0.72	5,080.00 - 6,685.00	0.00 - 1.04	1			1
		13,923.33 - 20,460.00	7,400.00 - 14,200.00	0.18 - 0.36	1,870.00 - 3,475.00	0.00 - 1.04		1		1
					3,475.00 - 5,080.00	0.00 - 1.04		661		661
						1.04 - 2.08		49		49
						2.08 - 3.13		12		12
						3.13 - 4.17		8		8
					5,080.00 - 6,685.00	0.00 - 1.04	34	673		707
						1.04 - 2.08		41		41
						2.08 - 3.13		8		8
					6,685.00 - 8,290.00	0.00 - 1.04	77	138		215
				0.36 - 0.54	1,870.00 - 3,475.00	0.00 - 1.04	1	3		4
					3,475.00 - 5,080.00	0.00 - 1.04	44	410		454
						1.04 - 2.08		8		8
						2.08 - 3.13		1		1
					5,080.00 - 6,685.00	0.00 - 1.04	438	631		1,069
						1.04 - 2.08	3	1		4
						2.08 - 3.13		3		3
					6,685.00 - 8,290.00	0.00 - 1.04	103			103
			14,200.00 - 21,000.00	0.18 - 0.36	3,475.00 - 5,080.00	0.00 - 1.04	2	44		46
						1.04 - 2.08		20		20
Poor strength	Actual strength	Coarse aggergates	Fine aggergates	W/(C+P)	Weight	AEA dose	1	2	3	Total
					5,080.00 - 6,685.00	0.00 - 1.04	13	102		115
						1.04 - 2.08		14		14
						2.08 - 3.13		1		1
					6,685.00 - 8,290.00	0.00 - 1.04	15	2		17
				0.36 - 0.54	3,475.00 - 5,080.00	0.00 - 1.04	47	75		122
						1.04 - 2.08		9		9
					5,080.00 - 6,685.00	0.00 - 1.04	266	34		300
						1.04 - 2.08	2	1		3
					6,685.00 - 8,290.00	0.00 - 1.04	105			105
	9,276.67 - 13,050.00	850.00 - 7,386.67	600.00 - 7,400.00	0.18 - 0.36	265.00 - 1,870.00	0.00 - 1.04			2	2
					1,870.00 - 3,475.00	0.00 - 1.04			3	3
				0.36 - 0.54	265.00 - 1,870.00	0.00 - 1.04			3	3
			7,400.00 - 14,200.00	0.18 - 0.36	3,475.00 - 5,080.00	0.00 - 1.04			1	1
		7,386.67 - 13,923.33	7,400.00 - 14,200.00	0.18 - 0.36	3,475.00 - 5,080.00	0.00 - 1.04		3	6	9
					5,080.00 - 6,685.00	0.00 - 1.04		4		4
				0.36 - 0.54	3,475.00 - 5,080.00	0.00 - 1.04	1			1
			14,200.00 - 21,000.00	0.18 - 0.36	6,685.00 - 8,290.00	0.00 - 1.04		2		2
		13,923.33 - 20,460.00	7,400.00 - 14,200.00	0.18 - 0.36	3,475.00 - 5,080.00	0.00 - 1.04		1		1
						1.04 - 2.08		2		2
					5,080.00 - 6,685.00	0.00 - 1.04	1	6		7
					6,685.00 - 8,290.00	0.00 - 1.04		2		2
				0.36 - 0.54	5,080.00 - 6,685.00	0.00 - 1.04	1			1
			14,200.00 - 21,000.00	0.36 - 0.54	5,080.00 - 6,685.00	0.00 - 1.04	3			3
yes	1,730.00 - 5,503.33	850.00 - 7,386.67	600.00 - 7,400.00	0.18 - 0.36	265.00 - 1,870.00	0.00 - 1.04			7	7
					1,870.00 - 3,475.00	0.00 - 1.04			2	2
					3,475.00 - 5,080.00	0.00 - 1.04			1	1
				0.36 - 0.54	265.00 - 1,870.00	0.00 - 1.04			8	8
						4.17 - 5.21			1	1
Poor strength	Actual strength	Coarse aggergates	Fine aggergates	W/(C+P)	Weight	AEA dose	1	2	3	Total
					1,870.00 - 3,475.00	0.00 - 1.04			3	3
			7,400.00 - 14,200.00	0.18 - 0.36	3,475.00 - 5,080.00	0.00 - 1.04			1	1
		7,386.67 - 13,923.33	600.00 - 7,400.00	0.18 - 0.36	1,870.00 - 3,475.00	0.00 - 1.04			8	8
					3,475.00 - 5,080.00	0.00 - 1.04			3	3
				0.36 - 0.54	1,870.00 - 3,475.00	0.00 - 1.04			6	6
					3,475.00 - 5,080.00	0.00 - 1.04			2	2
			7,400.00 - 14,200.00	0.18 - 0.36	1,870.00 - 3,475.00	0.00 - 1.04			1	1
					3,475.00 - 5,080.00	0.00 - 1.04		1		1
				0.36 - 0.54	1,870.00 - 3,475.00	0.00 - 1.04	2		5	7
					3,475.00 - 5,080.00	0.00 - 1.04	3	4	3	10
					5,080.00 - 6,685.00	0.00 - 1.04		2		2
			14,200.00 - 21,000.00	0.18 - 0.36	5,080.00 - 6,685.00	0.00 - 1.04	1			1
		13,923.33 - 20,460.00	7,400.00 - 14,200.00	0.18 - 0.36	3,475.00 - 5,080.00	0.00 - 1.04		18		18
					5,080.00 - 6,685.00	0.00 - 1.04	1	22		23
						1.04 - 2.08		1		1
					6,685.00 - 8,290.00	0.00 - 1.04	1	2		3
				0.36 - 0.54	3,475.00 - 5,080.00	0.00 - 1.04	15	25		40
						1.04 - 2.08		1		1
					5,080.00 - 6,685.00	0.00 - 1.04	12	68		80
						1.04 - 2.08		1		1
					6,685.00 - 8,290.00	0.00 - 1.04	4			4
			14,200.00 - 21,000.00	0.18 - 0.36	3,475.00 - 5,080.00	0.00 - 1.04		1		1
						1.04 - 2.08		2		2
					5,080.00 - 6,685.00	0.00 - 1.04		4		4
						1.04 - 2.08		1		1
				0.36 - 0.54	3,475.00 - 5,080.00	0.00 - 1.04	5	3		8
					5,080.00 - 6,685.00	0.00 - 1.04	4	1		5
					6,685.00 - 8,290.00	0.00 - 1.04	3			3
				0.54 - 0.72	1,870.00 - 3,475.00	0.00 - 1.04	1			1
	5,503.33 - 9,276.67	850.00 - 7,386.67	600.00 - 7,400.00	0.18 - 0.36	265.00 - 1,870.00	0.00 - 1.04			1	1
		7,386.67 - 13,923.33	600.00 - 7,400.00	0.18 - 0.36	3,475.00 - 5,080.00	0.00 - 1.04			1	1
			7,400.00 - 14,200.00	0.18 - 0.36	5,080.00 - 6,685.00	0.00 - 1.04		1		1
		13,923.33 - 20,460.00	7,400.00 - 14,200.00	0.18 - 0.36	5,080.00 - 6,685.00	0.00 - 1.04		1		1
					6,685.00 - 8,290.00	0.00 - 1.04		4		4
				0.36 - 0.54	6,685.00 - 8,290.00	0.00 - 1.04	1			1
Total							2,772	5,538	1,373	9,683

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Further Insights into EAML and Digital Twin for Future Gen Concretes

This section presents additional insights worthy of discussion that surfaced during the development of the proposed EAML digital twin framework.

Need for "quality" data

The use of approaches that heavily rely on ML and data, and hence the notion of data-driven approaches, such as that presented herein, requires the availability of good quality datasets. Such datasets are expected to be thorough, timely, and well documented. In practical scenarios, attaining such datasets can be expensive (both financially and timewise), which remains a crucial challenge to integrating ML-based frameworks into the concrete industry. As such, some of the available databases, including those showcased in this work, may not contain an exhaustive list of features and may be light on some items (i.e., specifics to the chemical composition of some raws, the lack of specification pertaining to material classes such as classes of Fly ash, etc.). Further, treatment of outliers needs improvements – as some outliers may reflect experimentally correct data. New approaches based on concrete research can come in handy to expand the concrete databases and enhance the anomaly detection and outlier treatment portion of the outlined approach.

However, one must realize that concrete manufacturers and producers generate a massive amount of such data on a daily basis that cover the full cycle of concrete life – most of which can be readily utilized in a digital twin. Noting the improvements in quality control and manufacturing of products in industries that adopt digital twin showcase the positive potential of integrating EAML into our industry [83]. A coalition between industry, academia, and other stakeholders can facilitate a smooth and timely integration of digital twinning [84].

Selecting proper algorithms and performance metrics

Another insight that is seen to be worthy of sharing revolves around the technical nature of EAML. For instance, a question may arise as to which algorithms and performance metrics can be used in developing such a framework? While the presented framework adopted three unsupervised algorithms (2 for anomaly detection and 1 for clustering) and four supervised algorithms (that are joined into an ensemble), the reader must realize that we do not yet have a standardized procedure to create digital twins [85]. Therefore, it is up to the users to create blueprints that work to their needs. The aforenoted is not to be seen as a limitation but as an opportunity that will enable us to create digital twins that are specific to the concrete industry as opposed to those commonly adopted in other industries. At the time of this write-up, the author believes that while there could be an optimal combination of algorithms and metrics that can be adopted, such a combination may only be realized through extensive trail-and-errors and investigation campaigns. This work presents the one step toward such direction and invites others to explore other combinations of algorithms and metrics. In all cases, the user is to strive to learn the advantages and limitations of the to-be-used algorithms to be able to properly gauge the merits of future digital twins. Particular attention should be paid to real-time modeling, resources needed (in terms of cloud services, coding software, etc.), and algorithm debugging, among others.

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Conclusions

This work presents a framework for integrating Explainable and Anomalous Machine Learning (EAML) into a digital twin to allow users to identify vulnerable concrete mixtures to extreme service loads or environmental conditions. This framework starts by applying anomaly detecting algorithms to spot suspicious data points. From then, an unsupervised clustering analysis takes place to group concrete mixtures of similar characteristics into unique clusters. These clusters are further explored to realize vulnerable mixtures to the phenomenon of interest (i.e., fire-induced spalling, chloride penetration, etc.). Once vulnerable mixtures are pinpointed, a supervised ML classifier is trained to spot such mixtures – thereby acting as a digital twin (or virtual assistance) to concrete mix designers/users. The properly validated classifiers are then augmented with explainability techniques to give users a glimpse into the decision-making process of Blackbox ML models – hence adding a new dimension of trust between ML and human users. The following list of inferences can also be drawn from the findings of this study:

- EAML-based digital twin presents an attractive, customizable, and scalable approach that may lead to further modernization of the concrete research and industry.
- Despite its merits, unsupervised ML remains underutilized. In this work, clustering analysis has been shown to reveal interesting observations from small and large datasets with regard to concrete mixture performance under working and extreme loading conditions.
- The application of explainable ML algorithms can turn Blackbox ML models into transparent and user-trustworthy models.
- A few challenges may arise with respect to integrating the proposed digital twin framework or ML-based approaches in general, such as the need for large and comprehensive datasets and proper ML applications. Fortunately, such challenges are expected to be overcome with continuous advancements in this field.

Data Availability

Some or all data, models, or code that support the findings of this study are available from the corresponding author upon reasonable request.

Conflict of Interest

The author declares no conflict of interest.

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