Leveraging Embedding Vectors of Aggregate Images for Particle Size Distribution Estimation and Concrete Compressive Strength Prediction

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Abstract: Accurate prediction of concrete properties, such as compressive strength, is essential for ensuring structural performance. Particle size distribution (PSD) and nature of aggregates are key components of concrete mixtures, significantly influencing their final compressive strength. This paper presents a novel approach that leverages embedding vectors extracted from images of aggregates using the DinoV2 model to efficiently predict compressive strength. DinoV2 is a state-of-the-art vision transformer that excels at generating high-quality embeddings for various visual tasks. In this study, the effectiveness of these embeddings is evaluated by using them to classify and estimate the PSD of aggregates on public datasets. Small neural models trained on these vectors achieved comparable accuracy to the best found fine-tuned ViT-16 model, demonstrating the potential of using embedding vectors for accurate PSD prediction. Building on these results, a new approach for predicting concrete compressive strength by combining embedding vectors with data on concrete mix components is explored. A small dataset of concrete mixtures was created. To mitigate the challenges of limited data, augmentation techniques were proposed to generate additional, realistic mix designs. An ablation study was performed, indicating promising results and highlighting the potential of this new approach for predicting other concrete properties.

1 INTRODUCTION

Among the properties of concrete, compressive strength is significant to evaluate. This property is essentially influenced by the principal components of its recipe, i.e. the quantities of water, cement and the used sources of aggregates. The latter differ in size (particle size distribution PSD) and type (recycled or natural). When dealing with natural aggregate concrete, it is possible to use semi-empirical formulas to approximate the compressive strength based on some parameters of the mix design. Using mixed or recycled aggregates introduces new factors, which makes it hard to use those formulas to predict the concrete strength.

This paper focus on the use of machine learning to train a model on various concrete recipes using different aggregate sources to predict compressive strength. The originality is to explore the potential of image embedding vectors of the aggregates for estimating concrete properties. To the best of our knowledge, no previous studies have integrated embedding vectors from aggregate images into concrete mix recipe data. However, successful work has been carried out to establish the PSD from aggregate images. Our study therefore begins by checking whether the embedding vectors we plan to use contain information relevant to aggregate images by means of estimating the PSD using them and comparing this approach with others. Figure 1 presents the two evaluations performed with the embedding vectors of the aggregate images.

The paper is organized as follows. After presenting the related works in section 2, section 3 presents the aggregates used in our work with their extracted embedding vectors. The two following sections answer the two questions that we deal with in this paper:

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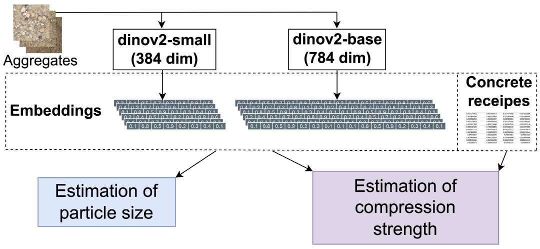


Figure 1: The two evaluations performed in this paper around the richness of embeddings vectors.

- Section 4 presents and discusses the performance of embedding vectors derived from aggregate images in estimating the particle size density (PSD). This section compares the proposed approach with existing techniques.
- Section 5 presents and evaluates the effectiveness of embedding vectors as supplementary features in predicting concrete properties. Additionally, this section details the small specialized dataset employed in our study, along with the augmented techniques developed to expand it.

Section 6 presents our conclusions, highlighting key results and outlining our future research directions.

2 RELATED WORKS

Previous research has demonstrated the feasibility of using aggregate images to predict PSD. Notable studies include Coenen et al.'s work (Coenen et al., 2022) using a dedicated CNN model (AggNet) to achieve 95.5% accuracy on the public dataset (Coenen, 2022). (Pasquier and Drissi, 2024) further explored this approach using pre-trained CNN models such as ResNet and transformers, achieving 97% accuracy, on the same dataset, by applying transfer learning and fine-tuning to a pre-trained ViT-16 model.

This paper, proposes a novel approach leveraging embedding vectors extracted from aggregate images using the DinoV2 model (Oquab et al., 2024). DinoV2 is a self-supervised learning model that has been trained on thousands of unlabelled images. Unlike previous studies relying on implicit feature extraction, our method explicitly extracts image embeddings and directly applied them to various tasks. For PSD estimation, a multi layer perceptron (MLP) model was created that takes these embedding vectors as input. The MLP was then trained to predict the PSD. To evaluate the approach, two publicly available datasets (Coenen, 2022) and (Coenen, 2023) were used, which aligns with our research objectives and provides a robust benchmark for comparison.

When it comes to estimating the concrete compressive strength, a time consuming experimental ”trial-and-error” approach can be used. Concrete specimens are cast in cylindrical or cubic molds of standard dimensions and the compressive strength (CS) measured at specific ages (e.g., 7 and 28 days). This approach was used in this study to build a custom dataset where the produced concrete not only uses natural aggregates but also recycled concrete aggregates (RA).

Various methods have been developed to estimate concrete compressive strength from the composition recipe. A method used in European countries is the so-called Bolomey's formula (Abdelgader et al., 2022). This semi-empirical equation considers the water-to-binder ratio, the average strength of the cement at a given age, a coefficient characterizing the aggregates and optionally the air content to estimate the compressive strength of a concrete with such a mix design. This equation provides reasonable predictions for normal concrete but lacks the finesse to be efficient with RA. Recycled concrete is produced with a fraction of its aggregate coming from crushed demolition waste, mostly concrete. Recycled aggregates tend to have physical properties much more variable than natural aggregates, thus making any prediction complex.

(Nithurshan and Elakneswaran, 2023) reviews predicting models of concrete compressive strength and presents the approaches and models used as well as the achieved accuracy. This review acknowledges the accuracy of Machine Learning (ML) models, even though it states that they may be difficult to interpret. Our study aims to use an ML approach to predict compressive strength of recycled aggregate concrete. Many studies compared a variety of ML models, including eXtreme Gradient Boosting (XGBoost), Random Forest, K-nearest Neighbors, Support Vector Regression, and Gradient Boosted Decision Trees (GBDT), to achieve this prediction. (Yuan et al., 2022) and (Ouyang et al., 2020) findings show that Random forest is a good tool for compressive strength prediction while (Zhang et al., 2023) demonstrated the superior predictive accuracy and generalization ability of GBDT. Similarly, (Hosseinzadeh et al., 2023) and (Wang et al., 2024) compared several ML models and found XGBoost to be the most accurate. These findings encouraged us to evaluate a decision tree technique, specifically XGBoost. While the datasets used in these studies may not have identical features, they all focus on the components of the concrete mix recipe. This is why none of these datasets is suitable for the present research, as they lack the necessary aggregate images for extracting embedding vectors alongside the recipe components. To address this, we developed a new, dedicated dataset. To assess the value of embedding vectors as additional features, we conducted an input ablation study, to investigate the benefits of incorporating them as additional features alongside traditional inputs.

3 AGGREGATE IMAGES AND THEIR EMBEDDING VECTORS

DinoV2 is a state-of-the-art self-supervised learning (SSL) framework designed for image representation learning. It is is trained on various large-scale unlabeled datasets. Its key output is an image embedding vector, which is a numerical representation that capture the semantic and visual information contained within an image. These embedding vectors can then be used for training models on different specific tasks. The backbone architecture used in DinoV2 is a Vision Transformer (ViT). Depending on the used ViT (ViT-Small, ViT-Base, ViT-Large and ViT giant), the embedding vectors are of different dimensional (384, 768, 1025 or 1535 respectivel).

For our study, we focused on the embedding vectors extracted from images of various aggregate sources used in concrete mixes. Our images are obtained by taking pictures in our laboratories. All images are homographically rectified to ensure consistency.

Ten distinct aggregate sources are used, including four natural aggregates and six recycled aggregates. These sources exhibited varying size distributions. Tables 1 and 2 provide the number of images for each recycled and natural source, respectively. The PSD ranges in mm are also provided for each source.

Table 1: Used recycled aggregate sources with their PSD range and the number of images.

Rec-1 0-6	Rec-2 4-22	Rec-3 0-4	Rec-4 4-16	Rec-5 0-16	Rec-6 0-16
96	71	94	31	80	102

Table 2: Used natural aggregate sources with their PSD range and the number of images.

Nat-7 0-4	Nat-8 4-8	Nat-9 8-16	Nat-10 16-32
87	80	96	86

For each aggregate source, every image was used to extract two embedding vectors using DinoV2. We selected 384 and 768 as our embedding dimensions, to achieve a favorable trade-off between representational power and computational efficiency, creating two multi-sets of embeddings: $\{EVS_i^{384}, i = 1..10\}$ and $\{EVS_i^{768}, i = 1..10\}$.

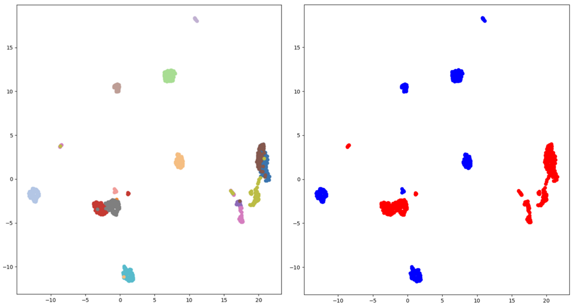


Figure 2: 2D UMAP visualization of EVS_i^{384}. Left - Embedding vectors / aggregate source: Each aggregate source is represented with a different color. Right - embedding vectors / aggregate type: Natural aggregates are in blue and recycled aggregates are in red.

Figure 2, shows the 2D UMAP visualization of the multi-set $\{EVS_i^{384}, i = 1..10\}$. On the left, the embedding vectors are colored according to their source origin, while the right the same embedding vectors are colored according to their type (recycled, natural). These visualisations, show that clusters corresponding to different aggregate origins and types were distinguishable in both cases. This confirms, that the embedding vectors carry relevant information on aggregates. However, two questions remain: Are these embedding vectors effective for estimating PSD, and can they help in predicting the properties of concrete? The two following sections answers these two questions.

4 PARTICLE SIZE DISTRIBUTION ESTIMATION

Aggregate particle size distribution, is a critical factor influencing the mechanical properties of concrete. Accurate estimation of PSD is essential for optimizing concrete mix designs. This section, explores the effectiveness of using embedding vectors extracted from aggregate images for PSD estimation and compare the presented approach with state-of-the-art methods, particularly focusing on the ViT-16 model as evaluated in (Pasquier and Drissi, 2024).

4.1 Evaluation Dataset

To ensure a fair and direct comparison with the ViT-16 model presented in (Pasquier and Drissi, 2024), the same publicly available datasets: the Visual Granulometry dataset (Coenen, 2022) and the Deep Granulometry dataset (Coenen, 2023) are used:

- The Visual Granulometry dataset is designed for a classification task and contains 900 images of aggregates, each labeled with its corresponding DIN 1045-2 standard granulometric class. There are nine classes in total, representing different grading curves or size distributions of the aggregates. Each class includes 100 images, ensuring a balanced dataset for classification.
- The Deep Granulometry dataset is intended for a regression task and consists of 1,650 images of coarse aggregate samples with particle sizes ranging from 0.1 mm to 32 mm. Each image is accompanied by the mass percentage of each particle size considered, following 33 different PSD.

These datasets provide a standardized benchmark for evaluating PSD estimation models. By using them, we ensure that our evaluation is consistent with previous studies and that any improvements or differences in performance can be attributed to the models themselves rather than discrepancies in the data.

4.2 Neural Networks

In our approach, we developped Multi-Layer Perceptron (MLP) models for the PSD estimation task. Each of the model maps the high-dimensional embedding vectors obtained from the DinoV2 model to respectively the granulometric classes (classification task: MLP_C_384/768) or particle size distributions (regression task: MLP_R_384/768).

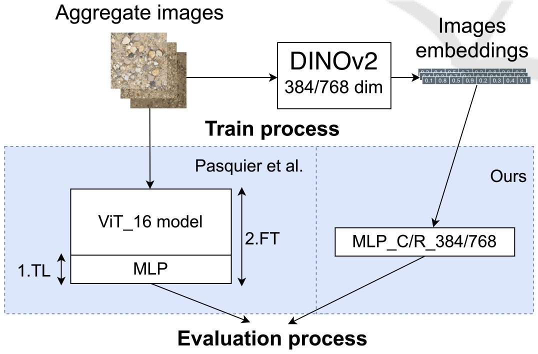


Figure 3: Illustrating the proposed approach compared to the existing one. TL = transfer learning, FT = fine tuning.

As illustrated in figure 3, the architecture of the proposed MLP_C/R_384/768 models varies depending on the dimensional of the embedding vectors. In each case we developed a model with four layers. For embeddings of dimension 384 extracted using the `facebook/dinov2-small` mode (resp. 768 extracted using the `facebook/dinov2-base` model), the MLP consists of:

- An input layer of size 384 (resp. 768)
- A hidden layer with 256 neurons (resp. 512) and ReLU activation.
- A second hidden layer with 128 neurons (resp. 256) and ReLU activation.
- An output layer corresponding to the number of granulometry classes (classification) or size bins (regression), with appropriate activation functions (softmax for classification, linear for regression).

The MLP models are trained using the Adam optimizer. For the classification task, we use the cross-entropy loss function; for the regression task, we use the mean squared error loss function. Early stopping is employed based on validation set performance to prevent overfitting.

4.2.1 Comparison with the Fine-Tuned ViT-16 Model

In the study conducted in (Pasquier and Drissi, 2024), the Vision Transformer model ViT-16 was evaluated for the task of PSD estimation and achieved state-of-the-art performance. They used transfer learning, freezing the feature extraction layers and training new fully connected layers on top. Extensive hyperparameter tuning, data augmentation, and fine-tuning were performed to optimize performance.

In comparison, our approach leverages the embedding vectors from DinoV2, allowing us to train relatively small MLP models directly on these embeddings. This simplifies the training process and reduces computational requirements, enabling rapid iteration and experimentation. Despite the simplicity of the proposed models, we achieve competitive performance in PSD estimation, as demonstrated in our experiments.

4.3 Experimental Setup

To ensure a fair and direct comparison with the ViT-16 model presented in (Pasquier and Drissi, 2024), we adopt the same experimental setup, using the same datasets and data splitting strategies. By mirroring the experimental setup described in this paper, we ensure that any differences in performance are due to the models themselves rather than experimental variations. Both studies use the same datasets, data splits, and evaluation metrics. While the authors performed extensive hyperparameter tuning and data augmentation, particularly for ViT-16, the proposed approach benefits from the efficiency of training on pre-extracted embedding vectors. The simplicity of the proposed MLP models allows for rapid experimentation without the need for extensive computational resources. Therefore the experimental procedure involves the following steps:

1. **Data Preparation:**
   - Datasets: for the classification task, the Visual Granulometry dataset (Coenen, 2022) is used; while the Deep Granulometry dataset (Coenen, 2023) is used for the regression task.
   - Embedding extraction: embedding vectors are extracted from each image using the DinoV2 model, as described in Section 4.2. To investigate the influence of dimensionality on performance, experiments were conducted with two different embedding vector sizes.
   - Data splitting: each dataset is split into training and test sets with an 80/20 ratio, identical to (Pasquier and Drissi, 2024). The training set is further split into training and validation subsets (80/20 split).
2. **Model Training and Evaluation:**
   - The fours MLP models (two classification models MLP_C_384/768 and two regression models MLP_R_384/768, each tailored to a specific embedding vector dimensionality) were trained as described in Section 4.2 on the training data, using the validation set with early stopping.
   - To account for variability due to random data splitting, the training process was repeated 10 times with different random seeds. This provides a more robust estimate of model performance.
   - Evaluation metrics: for classification, accuracy, precision, recall, and F1-score are used. For regression, mean absolute error (MAE) and root mean squared error (RMSE) are the two used metrics. The mean and standard deviation of these metrics are computed over 10 iterations.

4.4 Results and Discussion

The experimental results demonstrate that models trained on embedding vectors achieve competitive performance in classification and PSD estimation.

4.4.1 Classification Task

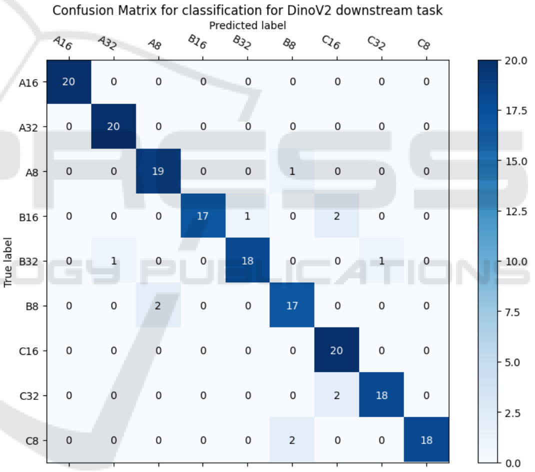
For the classification task on the Visual Granulometry dataset, the proposed MLP models (MLP_C_384 and MLP_C_768) achieved an accuracy of up to 93%, which is comparable to the 97% accuracy reported in (Pasquier and Drissi, 2024) using a fine-tuned ViT-16 model.

Table 3: Comparison of classification model accuracies.

Model	**ViT_16**	**MLP_C_384**	**MLP_C_768**
Accuracy	0.97	0.92	0.93

From the results presented in Table 3, we observe that using the 768-dimensional embeddings provides a slight improvement in accuracy compared to the 384-dimensional embeddings. Although the ViT-16 model achieves higher accuracy, our MLP models trained on DinoV2 embeddings perform competitively with significantly reduced complexity and training time.

Figure 4 shows the confusion matrix for the MLP_C_384 model trained on 384-dimensional embeddings. The confusion matrix indicates that the model performs well across most classes, with minor misclassifications occurring between similar granulometry classes. This suggests that the embedding vectors effectively capture the visual features necessary for distinguishing between different aggregate sizes.



	A16	A32	A8	B16	B32	B8	C16	C32	C8
A16	20	0	0	0	0	0	0	0	0
A32	0	20	0	0	0	0	0	0	0
A8	0	0	19	0	0	1	0	0	0
B16	0	0	0	17	1	0	2	0	0
B32	0	1	0	0	18	0	0	1	0
B8	0	0	2	0	0	17	0	0	0
C16	0	0	0	0	0	0	20	0	0
C32	0	0	0	0	0	0	2	18	0
C8	0	0	0	0	0	2	0	0	18

Figure 4: Confusion matrix for the MLP model trained on 384-dimensional embedding vectors.

4.4.2 Regression Task

For the regression task on the Deep Granulometry dataset, the models were evaluated using MAE and RMSE metrics. The MLP models trained on embedding vectors achieved an MAE of 1.06% and an RMSE of 1.51%, while the ViT-16 model achieved an MAE of 0.59% and an RMSE of 0.93%. These results are summarized in Table 4.

While the ViT-16 model demonstrates better performance in terms of MAE and RMSE, our MLP models still achieve respectable results, especially considering the simplicity of the model and reduced computational requirements. The regression results compare favorably with other models evaluated in

Table 4: Regression model performance comparison.

Model	MAE (%)	RMSE (%)
ViT_16	0.59	0.93
AGGNet	1.15	1.62
MLP_R_384	1.18	1.62
MLP_R_768	1.06	1.51

(Pasquier and Drissi, 2024), such as AggNet and other CNN-based architectures, which reported higher errors than ViT-16. The AggNet model achieved an average MAE of 0.73% and an RMSE of 1.15% on the Deep Granulometry dataset, which is close to our MLP models' performance. This indicates that our approach is still competitive with specialized models designed for PSD estimation.

Moreover, (Pasquier and Drissi, 2024) highlighted that averaging predictions over multiple images of the same aggregate mixture can significantly improve the accuracy of PSD estimation. By averaging, even the worst individual predictions become much closer to the ground truth. This suggests that our approach could similarly benefit from such averaging techniques, potentially narrowing the performance gap with ViT-16.

5 COMPRESSIVE STRENGTH ESTIMATION

While the previous section demonstrated that embedding vectors capture information about aggregates, it remains to be determined whether this information can be effectively used to estimate concrete properties.

5.1 Custom Dataset of Concrete Mix

Usually cement, water and aggregates proportions are used as input data to the ML models to predict the compressive strength as in the public dataset (Yuan et al., 2022) . As we focus our research on the impact of incorporating embedding vector of aggregate images while predicting compressive strength of a concrete, pre-existing datasets are unsuitable for our study. Therefore, we build a custom dataset.

First, we designed a reference concrete mix able to reach the C30/37 compressive strength class, containing a minimal amount of 5% by weight of each of the aggregate sources and a total of 55% of RA in the aggregate fraction. The adequate effective water-to-binder ratio was set to 0.49. The subsequent mixes contained between 40% and 70% of recycled aggregate, coming from different RA sources. In all recipes, the granulometric curve of aggregates mix followed the distribution of a Füller curve, with Dmax = 32 mm. In addition, the water absorption WA24 of each of the aggregate sources was measured according to SN EN 1097-6:2014. This allowed us to take into account the water that would be absorbed by the aggregates during mixing. Therefore, extra water was used in the mix to aim for the established effective water-to-cement ratio. Only the superplasticizing admixture dosage was slightly adapted to the total RA content to reach a workability similar to the reference mix. For each mix design, we cast three 150 mm cubes and four 150/300 mm cylinders to be tested at 28 days for compressive strength.

Given the time-intensive process of concrete production and testing, only 23 unique concrete mix recipes were generated. We fixed the quantities of cement and water in all the mix designs, allowing us to study isolated effects of aggregate properties (type, PSD and amount) on compressive strength. The compressive strength (CS) of each mix was subsequently measured at 28 days. The measured compressive strength values fall within the range of 35.2 to 46.5 MPa, with an average of 39.2 MPa, a median of 39, and a standard deviation of 3 MPa.

The variability in our dataset is due to the different aggregate sources employed, all other elements being held constant. These sources are selected from the set of 10 distinct aggregates presented in section 3. The main uncertainty on the CS prediction, comes from the use of recycled concrete aggregates which change the properties of the recipe in an unpredictable way. This is why we used the same 4 sources of natural aggregates in practically all recipes, changing only their proportion in each mix design, and thus measure the impact of recycled aggregates. On the other hand, mix designs use different combination of the 6 sources of recycled aggregates as illustrated in figure 5. Each of these 6 sources is used in approximately the same number of recipes as it is shown in figure 6.

Data collected for each of the 23 recipes is composed of two main variable components R_{we} and R_{CS} (Figure 7 left side):

- R_{we} is a vector of 10 values indicating the weight of aggregates (kg/m^3) for each of the 10 sources used in the recipe. A value is set to 0, for the unused sources.
- R_{CS} is a vector of 7 values of the measured compressive strength on a cylinder (MPa) at 28 days. For each mix recipe, the mean value of the 7 compressive strength is taken as the compressive strength.

Besides, constant information directly related to the 10 used aggregates sources are available (Figure 7 right side):

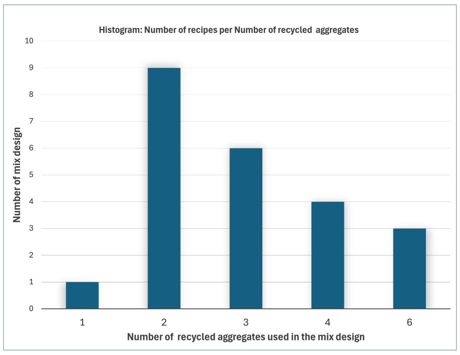


Figure 5: Histograms of number of recipes per number of used aggregates.

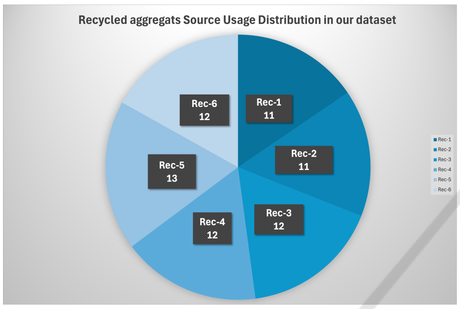


Figure 6: Recycled aggregates source usage distribution over the 23 mix design of the dataset.

- R_{WA24} is a constant vector of 10 values related to the Water absorption WA24 (l/m^3) of each aggregate source.
- EVS_i^{384}, EVS_i^{768}, EVS_i^{384PCA}, EVS_i^{768PCA} : the 4 sets of embedding vectors extracted for the i-th aggregate sources. The two last ones are generated by applying Principal Component Analysis (PCA) with a 5-dimensional projection to the EVS_i^{384} and EVS_i^{768} respectively.

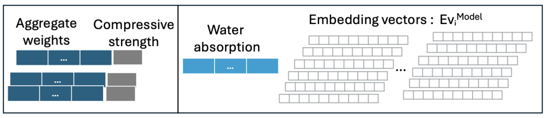


Figure 7: Left: Aggregate weights and compressive strengths for each of the 23 mixes design. Right: Data shared by all mixes.

5.2 Dataset Configurations

We prepared various dataset configurations for our study. The *baseline* configuration used only the 23 starting data points. The accuracy of ML models is directly related to the size of the training dataset. (Ouyang et al., 2020) demonstrated that a minimum of thousands data points is required to achieve maximum accuracy with the Random Forest technique (RF). Recognizing the limited size of our dataset, we proposed a novel data augmentation approach to expand it to a reasonable size. The *AUG* dataset is the dataset obtained by applying the data augmentation techniques. We also explored configurations with added water absorption data (*WA* datasets) and configurations incorporating embedding vectors (*ENR* datasets).

5.2.1 Baseline Configuration

This is the smallest dataset, as it is composed of 23 vectors of 10 values indicating the weight of the used aggregates and the mean of the measured CS.

5.2.2 Augmented Data Configuration

To expand our small initial dataset, we propose a data augmentation techniques to generate additional, realistic mix design, similar to approaches employed in image processing (Shorten, 2019).

Weight Augmentation. The goal of this augmentation is to slightly change the value of each $R_{we,i} = (w_{1,i}, \ldots w_{10,i})$ where $w_{j,i}$ is the weight of aggregates used from the j-th source, under the three following constraints:

- The overall weights of aggregates $W_{T,i}$ is constant between the original data and the augmented one.
- Only the weights of the used sources in a recipe is changed (not adding new sources).
- Uncertainty in weight measure is about ± 10% of the weight, corresponding to ± 100g for 1 kg which is translated to add to each used $j-th$ aggregates an $\varepsilon_j = random.uniform(-0.1, 0.1)$.

This leads to obtain $R^{aug}_{we,i} = (w_{1,i} + \delta_1 * \varepsilon_1, \ldots, w_{10,i} + \delta_{10} * (\varepsilon_{10}))$ where $\delta_i = 0$ if the i-th aggregate source is not used and 1 otherwise and to ensure the three constraints,the equation 1 must be respected:

$$\sum_{i=1}^{10} \delta_i * \varepsilon_i = 0 \tag{1}$$

Using this approach , several different $R^{aug}_{we,i}$ can be generated from an initial $R_{we,i}$.

Compressive Strength Augmentation. The goal of this augmentation is to create more realistic compressive strength values based on the existing ones. This augmentation is based on the following assumption: the compressive strength of the concrete follows a log-normal distribution (Matthews et al., 2023).

Each raw data, has 7 values : R_{CS} of the 7 measured compressive strengths. To augment the compressive strength value, we then generate $Cs^{'} = logNormal(\mu, \sigma)$ where

$$(\mu = \frac{1}{7}\sum_{i=1}^{7} log(s_i), \sigma = \sqrt{\frac{\sum_{i=1}^{7}(log(s_i) - \mu)^2}{7}}) \quad (2)$$

5.2.3 Enriched Configuration with Water Absorption

Our interest is to analyze the impact of using water absorption information while computing the compressive strength. Therefore, we prepared configurations where the data are enriched with the water absorption data. To avoid adding 10 constant water absorption values to all the rows of our input data, variability is introduced by applying water absorption augmentation defined as follow.

Water Absorption Augmentation. The goal of this augmentation is to create more realistic water absorption values based on the existing ones. This augmentation is based on the following assumption : the measure of the water absorption for each aggregate source is precise at +/- 10%.

Thus, given the Water absorption value A_i for the i-th aggregate source, we simple generate $A_i(1+\varepsilon_i)$ where each $\varepsilon_i = random.uniform(-0.1, 0.1)$.

5.2.4 Enriched Configuration with Embedding Data

Another important configuration in our study, is to enrich the raw data with visual embedding vectors. The parameter for this configuration is the model M_j used to create the embedding sets model: $EVS_i^{M\text{-}j}$, with M_j in [Dummy, 384, 768, 384 PCA, 768 PCA] and i=1..10 for the 10 used aggregate sources.

The Dummy vectors in EVS_i^{Dummy} were created with randomly generated values within the min-max range of real 384-dimensional embedding vectors. This dataset, having values similar to that of real embedding vectors, is used to assess the impact of real embedding vectors on the compressive strength prediction.

To enrich a raw data according to a model M_j, with the visual embedding vectors, 10 embedding vectors are added, randomly selected from the 10 sets: $EVS_i^{M\text{-}j}$. The variability in the embedding vectors directly comes from the variability in the images of each of the aggregate sources.

5.3 Experimental Setup

5.3.1 Metrics

To evaluate our pipeline, we propose two metrics which provide complementary information about the model's performance. We compute the RMSE along with the MAE because the RMSE penalizes more the large errors than the MAE. It is sensitive to outliers which is less the case of the MAE measure. We use the RMSE instead of the MSE because it is more interpretable as it is in the same unit as the ground truth mass percentage vector.

5.3.2 Models

We are interested in evaluating the benefit of using embedding vectors for the compressive strength evaluation. We first choose a basic model for this regression task: "Simple Linear Regression". Then, and as presented is section 2, we used "XGBoost" (eXtreme Gradient Boosting). This is a non linear model. It creates a series of decision trees, each of which learns from the errors of its predecessors. The final prediction is an ensemble of the predictions from all the trees. Scikit-learn (Pedregosa et al., 2011) provided the implementations for the models used in this study.

5.4 Experimental Design

To evaluate the performances of the different models, we use an identical experimental setup for all of them except for the baseline where all the original raw data were used without augmentation or enrichment of data. A K-Fold with 5 folds is used for the prediction on the original 23 inputs. The training set contains 80% of the data (18 recipes) and the test set 20% (5 recipes). The training set is used for the training and the cross-validation and the test set is used to evaluate the model.

For all the others experiments, 5 different seeds are used to split the data into train/test set using scikit-learn's `train_test_split` function. This simulates the 5-fold cross-validation and guarantees that we test our model on different test sets. We then report the average and standard deviation of the test errors across the five iterations.

Figure 8 illustrates the methodology used for the evaluation. For each of the five experiments, we first split the dataset into a training and test set with a ratio of 50% (11 recipes) and 50% respectively (12 recipes), the latter being only used for the final evaluation of each model in each ablation configuration of the inputs. Before training, a step of dataset preparation is done to create the different configuration of

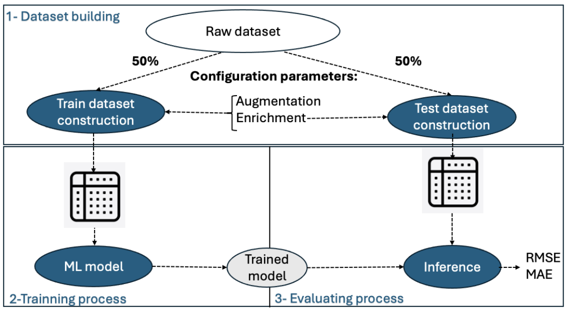


Figure 8: Train and test sets preparation giving the raw data and the description of the needed configuration: with or without embedding vectors etc.

input data. Here are the details on the 13 datasets that are created to conduct our study:

- Baseline: 23 original input raw data each with 10 features.
- AUG: each original input of the train set is augmented by 100 copies (The number 100 was chosen based on our experiments) using our weight and cs augmentation approach. This resulted in a total of 11 * 100 = 1100 input rows. Each input row has 10 features.
- AUG & WA : water absorption information is added to the AUG data set. The water augmentation function is used to avoid adding a constant vector. Each input row has 20 features.
- AUG & ENR - [Dummy, 384, 768, 384 PCA, 768 PCA] : each original train data is augmented by 100 copies and ten embedding vectors are added, each one corresponding for each aggregate sources. Each input row has (10 + 10*embedding dimension) features.
- AUG & WA & ENR - [Dummy, 384, 768, 384 PCA, 768 PCA] : which combines augmentation with enrichment of water and visual embeddings. Each input row has (20 + 10*embedding dimension) features.

All the experiments were conducted with the 3 proposed models: the Linear Regression with the default parameters from scikit-learn (Pedregosa et al., 2011) , a XGBoost and a XGBoost with early stopping. The XGBoost model is used with a maximum depth of 2 and 100 estimators. The early stopping is based on the MAE with a patience of 5 rounds and the same other hyperparameters as the XGBoost model.

5.5 Results and Discussion

Experiments were conducted following the methodology presented in section 5.4. We were interested in answering the following questions:

Q1. Do we need to employ a more complex model than linear regression, given that we only varied aggregate sources while maintaining constant water and cement quantities?

Q2. Does the implementation of data augmentation as suggested in this study make sense and is it beneficial?

Q3. Do embedding vectors enhance prediction results?

Q4. Does the dimensional of embedding vectors impact the outcomes?

Figure 9 illustrates the Mean Absolute Error (MAE) achieved by the three used models across the different dataset configurations. The results show that the linear regression model (blue curve) underperforms with a big error value compared to XGBoost models which consistently enhance predictions, providing an affirmative answer **A1**, to **Q1**. Moreover, the figure highlights that the XGBoost model with early stopping (green curve) is the best model among the three tested models.

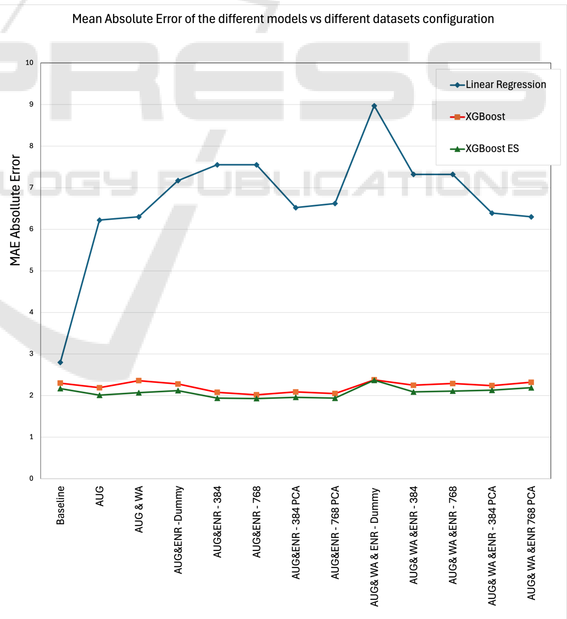


Figure 9: Visualization of the MAE of the predicted values on the different test datasets. The green curve is the result of the XGBoost early stop. It has the best results.

To address the remaining three questions, we focus on the results presented in Figure 10 for Mean Absolute Error (MAE) and Figure 11 for Root Mean Squared Error (RMSE), specifically considering the best model: XGBoost model with early stopping.

In these figures, we not only consider the mean

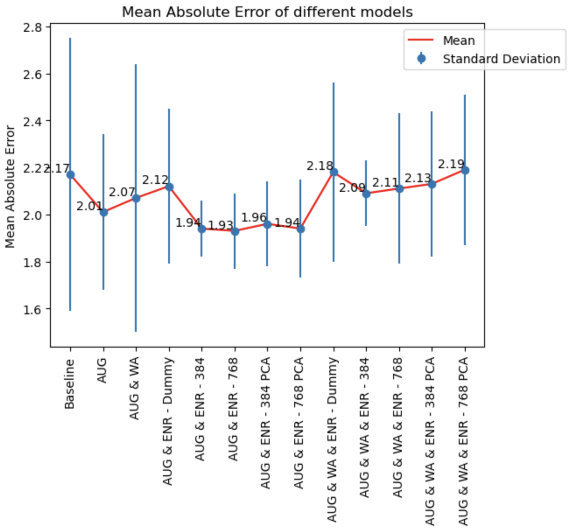


Figure 10: Visualization of the results on the test set for all the different experiments for the XGBoost with early stopping on the MAE. The best results are obtained by the 4 configurations including AUG and ENR.

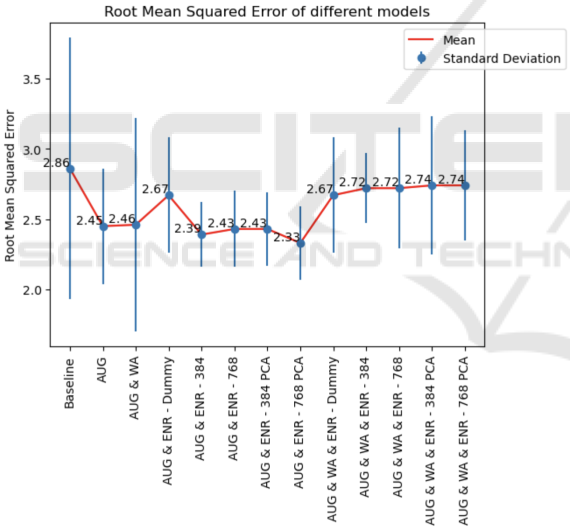


Figure 11: Visualization of the results on the test set for all the different experiments for the XGBoost with early stopping on the RMSE. The best results are obtained by the 4 configurations including AUG and ENR.

values of the error but also the standard deviation, indicating the model's reliability. Analysing the results, we draw the following answers:

A2. The augmentation strategy for weights and compressive strength, as proposed in this study is beneficial and improved the results on the mean error and on the standard deviation.

In contrast, augmenting the data with water absorption data, using the proposed function, has a negative impact on performance in all dataset configuration with WA. Therefore, it is advisable to exclude this feature from the input variables.

A3. The incorporation of embedding vectors enhances the prediction results (an improvement of 4% between AUG and AUG&ENR-768 on the avergae MAE), this is seen in the results of all the configurations including ENR in their label (excluding configuration with WA and Dummy). In addition, we can clearly see an improvement of the standard deviation which suggests that the models are more reliable than the one using only the AUG dataset.

To further validate the beneficial impact of using embedding vectors, we created configuration with the use of the EVS_i^{Dummy} instead of the real embeddings vectors. This resulted in degradation of performance, confirming the positive impact of using visual embedding vectors.

A4. The choice of the embedding dimension, 384 or 768, has little impact with a minimal effect on performance. More over, using either 384-dimensional embeddings and even its 5-dimensional PCA reduction still yields comparable performance.

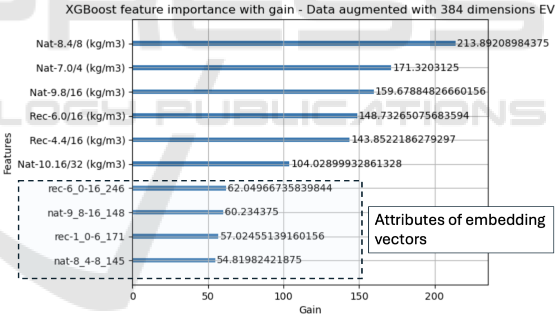


Figure 12: XGBoost feature importance with gain on the AUG & ENR 384 configuration dataset. The final four features are vector embedding attributes.

A final key observation is that embedding vectors are not the primary factors influencing the XGBoost model's ability to predict concrete compressive strength. As illustrated in Figure 12, the proportion of aggregates in the concrete mix is the more significant determinant for compressive strength, which aligns with expectations. Still, visual embedding vectors improves the prediction, and the four last influencing factors are particular attributes of embedding vectors.

6 CONCLUSIONS

The effectiveness of visual embedding vectors for predicting both aggregate particle size distribution and concrete properties was investigated. Our findings demonstrate that embedding vectors, when used to train simple MLP (Multi-Layer Perceptron) models, can accurately classify aggregates. The achieved accuracy is comparable to that obtained with more specialized or complex models. Therefore, when dealing with new aggregate sources, only their images need to be taken, the corresponding embedding vectors generated, and the model retrained with these new vectors.

In addition to aggregate classification, the potential of embedding vectors to help predict one of the key properties of concrete was explored. To evaluate this, we contructed a custom dataset and a novel estimation approach was developed. Due to the high cost and time investment associated with each concrete formulation, a limited dataset was built, focusing solely on the variability of aggregate proportions while keeping water and cement quantities constant. To ensure the validity of the findings, the limited dataset was intentionally split in half, training the models on one portion and reserving the other for evaluation on unseen data. This choice led to a very small training set size, so data augmentation techniques were proposed and implemented to expand the training dataset with realistic synthetic new samples.

Through extensive experimentation, we validated the effectiveness of the proposed approach. The results showed that embedding vectors are useful in predicting concrete compressive strength. The proposed augmentation techniques were also validated. The best results were obtained when embedding vectors were added to the input raw data and the training dataset was augmented using the weight and compressive strength augmentation techniques. The best model can predict concrete compressive strength with an MAE error of 1.94 MPa and an RMSE of 2.39 MPa. Considering that this is less than half of the 5 MPa standard deviation assigned to compressive strength when statistical data is missing (Matthews et al., 2023), it can be stated that the approach shows promising results despite the limited dataset. Further exploration of hyperparameter tuning for both particle size and compressive strength prediction processes is now feasible to obtain the best parameters for each model.

A limitation of our study is the size and scope of the dataset, which included a limited number of collected data points and variations in mix recipes. Expanding the dataset to include other key ingredients such as water content and cement content and its type, would be an interesting future direction.

As future work, and to further confirm our findings, we propose to expand our study to the other properties of concrete e.g. workability, early strength, carbonation resistance, etc. It would also be beneficial to evaluate the proposed data augmentation techniques on conventional datasets from the literature to validate their contribution. Finally, we also intend to explore the use of the visual embedding vectors to classify mixed aggregates and again use them in the process of estimating the properties of concrete, that has been manufactured using these mixed aggregates.

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