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Data-Driven Prediction of Concrete Strength Using Alternative Aggregates and Binders

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Abstract
The mechanical performance of concrete is fundamentally governed by the complex interactions between its constituent materials, necessitating precise modeling to ensure structural integrity and sustainability. This study develops a robust data-driven framework to predict two critical performance indicators: Compressive Strength (CS) and Split Tensile Strength (STS). The research utilizes an experimental dataset comprising 30 distinct mix designs characterized by the partial replacement of traditional constituents with industrial by-products and alternative aggregates. Specifically, the influence of Fly Ash (as a cement replacement), Foundry Sand (as a fine aggregate replacement), and Rounded Aggregates (as a coarse aggregate replacement) was evaluated across varying proportions.To model these relationships, the study evaluates the predictive accuracy of a diverse suite of machine learning (ML) algorithms, ranging from linear benchmarks to advanced ensemble techniques. The models investigated include Multiple Linear Regression (MLR), Ridge Regression, Support Vector Regression (SVR-RBF), and several tree-based ensembles, namely Random Forest, Extra Trees, Gradient Boosting, XGBoost, and LightGBM. Model reliability was quantified using four key statistical metrics: the coefficient of determination (R^2), Root Mean Square Error (RMSE), Mean Absolute Error (MAE), and Mean Absolute Percentage Error (MAPE).The findings demonstrate that ensemble-based models, particularly XGBoost and LightGBM, offer superior predictive capabilities, effectively capturing the non-linear effects of varying Fly Ash, Foundry Sand, and Rounded Aggregate content on the concrete's strength profile. By accurately forecasting CS and STS through a unified computational approach, this study provides a powerful tool for mix design optimization, reducing the reliance on extensive laboratory trials and accelerating the development of sustainable, high-performance concrete.
Keywords *Compressive Strength; Split Tensile Strength; Fly Ash; Foundry Sand; Rounded Aggregates; Machine Learning; XGBoost; Concrete Mix Optimization; Sustainable Construction Materials; Predictive Modeling.*

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I. Introduction

Concrete stands as the cornerstone of global infrastructure due to its exceptional versatility and high compressive strength. However, the surge in urban development has catalyzed a rapid depletion of natural sand resources and an escalation in carbon emissions tied to cement production[1]. Addressing these environmental challenges necessitates a shift toward sustainable construction practices, primarily through the integration of industrial byproducts that can maintain structural integrity while reducing the ecological footprint[2][3]. Among these, **Fly Ash (FA)**, **Foundry Sand (FS)**, and **Rounded (Pebble) Aggregates** have emerged as promising substitutes for cement, natural fine aggregates, and crushed coarse aggregates, respectively, offering a dual benefit of waste mitigation and performance enhancement[1][4].

Fly ash, a byproduct of coal combustion, exhibits significant pozzolanic properties due to its rich silica and alumina content[1][2]. When introduced into a concrete matrix, it reacts with calcium hydroxide to produce additional calcium silicate hydrate (C-S-H) gel, which densifies the microstructure and bolsters long-term strength[4][5]. Similarly, foundry sand—a byproduct of metal casting—shares physical characteristics with natural fine aggregates. Its high silica content and uniform grading can improve particle packing, though its effectiveness is highly dependent on the replacement ratio[1]. Furthermore, the inclusion of rounded aggregates (pebbles) provides a different mechanical interlocking mechanism compared to angular crushed stone, impacting both the workability and the **Split Tensile Strength (STS)** of the mix[3][5].

The simultaneous incorporation of FA, FS, and Rounded Aggregates creates a complex, nonlinear relationship between the mix design and the resulting mechanical properties. Factors such as the water-cement ratio and the specific replacement percentages interact in ways that traditional empirical models often fail to capture accurately[4][6]. Conventionally, **Compressive Strength (CS)** and **STS** are determined through destructive experimental testing, a process that is notoriously time-consuming and resource-intensive[5].

To circumvent these limitations, the field of concrete technology has increasingly turned toward Machine Learning (ML) as a robust predictive framework[6]. Unlike classical regression, ML algorithms can learn from extensive datasets to model the intricate dependencies between material proportions and strength outcomes[5][6]. The general predictive function for such models is defined as:
The general predictive function for such models is typically defined as:

$$\widehat{f_c} = ML\,(C, FA, Fine_{agg}, FS, CS, RA)$$

Where $\widehat{f_c}$ represents the predicted CS or STS, and the input variables include cement (C), fly ash (FA), natural fine aggregate ($Fine_{agg}$), foundry sand (FS), coarse aggregate (CA), and rounded aggregate (RA). By leveraging advanced algorithms, it is now possible to optimize these green concrete mix designs with minimal trial-and-error experimentation[4][6].

This study is about bringing concrete testing into the digital age. By using computational intelligence, we're creating a reliable way to forecast the strength of eco-friendly mixes containing recycled foundry sand and fly ash. By integrating these sustainable materials with cutting-edge ML techniques, this research supports the transition toward an efficient, data-driven, and environmentally responsible construction industry.

The integration of industrial by-products and alternative aggregates in concrete is a critical step toward sustainable construction. **Siddique**[1] emphasized the environmental benefits of utilizing waste materials, such as foundry sand and coal ash, to reduce the carbon footprint and manage industrial waste effectively. Building on the fundamental properties of concrete, **Neville (as reviewed by Krauss and Paret)**[2] provides the essential framework for understanding how varying aggregate shapes—such as rounded versus angular—affect the internal stress distribution and the resulting compressive and tensile capacities.

The chemical contribution of these materials is equally vital; **Naik and Moriconi**[3] highlighted that environmental-friendly concrete using recycled materials like fly ash not only supports sustainability but can also enhance long-term durability through refined pore structures. This is echoed by **Khatib**[4], who noted that the sustainability of construction materials hinges on the successful replacement of virgin resources without compromising the mechanical performance of the structure.

Predicting the properties of these complex, sustainable mixes has led to a surge in machine learning (ML) applications. **Yeh**[5] pioneered the use of Artificial Neural Networks (ANNs) to model the nonlinear relationships in high-strength concrete strength, demonstrating that computational models could significantly outperform traditional linear regression in handling multi-component mixes. More recently, **Thapa**[6] reviewed modern ML approaches, confirming that as datasets become more complex—incorporating variables like fly ash and diverse aggregate types—advanced algorithmic suites are required to maintain predictive accuracy. This study builds upon these foundations by employing an ensemble of ML techniques to specifically analyze the synergistic effects of Fly Ash, Foundry Sand, and Rounded Aggregates on the mechanical behavior of concrete.

II. Materials

Cement

Cement is essentially the glue that holds concrete together, giving it the strength to set and harden. For this study, we chose 53-grade Ordinary Portland Cement as our binder. To ensure everything was up to code, we put it through a rigorous battery of tests following IS 4031-1988 and confirmed it meets all the standard requirements of IS 12269-1987.[7]

Table 1 Physical properties of OPC 53 grade cement.

Properties	Results
28 days Compressive strength	53 N/mm^2
Initial setting time	40 Minutes
Final setting time	240 Minutes
Fineness	2890 m^3/Kg
Soundness	2.7

Water
Water is what triggers the hardening process in cement. For the best results, we use pure, clean water and measure it carefully—getting that balance right is the secret to making the concrete as strong as possible.[7]

Chemical Admixture
Perma Plast-SL allows for a significant reduction in water content while maintaining the workability of the mixture. This leads to a denser and stronger concrete by increasing the compressive strength and reducing porosity.[7]

Table 2 Properties of Perma Plast-SL.

Properties	Results
Colour	Dark Brown
Specific gravity (G)	1.15
Chloride Content	0.00%
Nitrate Content	0.00%

Aggregate
Aggregates act as the structural framework of the concrete matrix. Whether you're using crushed stone, sand, or recycled slag, these materials provide the bulk and compressive strength needed for a solid composite. To ensure a high-performance mix, the aggregates must be clean—free of silt, clay, or organic impurities that could interfere with the bond between the paste and the stone. Ultimately, choosing well-graded, clean aggregates is what determines the concrete's workability, long-term durability, and overall structural integrity.[8]

Fine Aggregate (FA)
The coarse aggregate represents the most chemically stable and least permeable phase of the concrete matrix. By utilizing angular, machine-crushed 10 mm aggregates, we maximize the mechanical interlock between particles, which significantly bolsters compressive strength and mitigates issues like drying shrinkage or creep. Because the surface area and shape of these stones dictate the mix's water demand and workability, we strictly evaluated their physical properties—including specific gravity and voids per IS 2386–1963 (Part 3) to ensure they met the rigorous demands of our structural application.[7][8]

Table: - 3 Properties of sand of zone –II.

Properties	Results
Specific gravity (G)	2.67
Bulking	34.30%
Water absorption (WA)	1.20%
Density (q)	1610 Kg/m^3

Coarse Aggregate (CA)
The coarse aggregate component of concrete is the most durable and least permeable. It is enhancing the durability and strength of concrete. The use of angular, machine-crushed aggregates with a 10 mm size helps in preventing issues like drying shrinkage and dimensional changes. These aggregates impact the workability, strength, and water requirements of the mix. Tests, as per IS 2386–1963 Part 3, were conducted to assess their properties, confirming their suitability for the intended concrete applications.[7]

Table: - 4 Properties of coarse aggregate.

Properties	Results
Specific gravity (G)	2.74
Aggregate crushing value	29.32%
Water absorption (WA)	0.8%
Density (q)	1780 Kg/m^3

Foundry sand (FS)

Foundry sand is a byproduct of the ferrous and nonferrous metal casting industries, which consists primarily of silica sand. For the purpose of this study, the foundry sand was brought from a metal casting facility located near Kalol, Gujarat. Some tests were conducted to determine properties such as specific gravity, water adsorption and density.[7]

Table: - 5 Properties of Foundry Sand.

Properties	Results
Specific gravity (G)	2.74
Water absorption (WA)	0.00%
Density (q)	1570 Kg/m3

Concrete mix proportions

high-strength concrete, M80, was designed in accordance with relevant mix design guidelines. The target compressive strength for the control mix was achieved based on standard design procedures. In this study, the conventional concrete mix was modified by incorporating sustainable material replacements. Cement was partially replaced with fly ash, natural sand was replaced with foundry sand, and coarse aggregate was replaced with pebble aggregate at varying proportions. Different replacement levels were considered to evaluate their influence on compressive strength. The detailed mix proportions corresponding to each variation are presented in Table 6.

Table 6:- Proposed Mix for different propositions.

Mix Design	Cement	Fly Ash	Fine Aggregate	Foundry Sand	CA	Rounded Aggregate
Mix 1	100%	0%	100%	0%	100%	0%
Mix 2	90%	10%	100%	0%	100%	0%
Mix 3	80%	20%	100%	0%	100%	0%
Mix 4	75%	25%	100%	0%	100%	0%
Mix 5	100%	0%	90%	10%	100%	0%
Mix 6	100%	0%	80%	20%	100%	0%
Mix 7	100%	0%	70%	30%	100%	0%
Mix 8	100%	0%	60%	40%	100%	0%
Mix 9	100%	0%	100%	0%	95%	5%
Mix 10	100%	0%	100%	0%	90%	10%
Mix 11	100%	0%	100%	0%	85%	15%
Mix 12	100%	0%	100%	0%	80%	20%
Mix 13	90%	10%	90%	10%	95%	5%
Mix 14	90%	10%	90%	10%	90%	10%
Mix 15	90%	10%	80%	20%	95%	5%
Mix 16	90%	10%	80%	20%	90%	10%
Mix 17	90%	10%	70%	30%	95%	5%
Mix 18	90%	10%	70%	30%	90%	10%

Mix 19	80%	20%	90%	10%	95%	5%
Mix 20	80%	20%	90%	10%	90%	10%
Mix 21	80%	20%	80%	20%	95%	5%
Mix 22	80%	20%	80%	20%	90%	10%
Mix 23	80%	20%	70%	30%	95%	5%
Mix 24	80%	20%	70%	30%	90%	10%
Mix 25	75%	25%	90%	10%	95%	5%
Mix 26	75%	25%	90%	10%	90%	10%
Mix 27	75%	25%	80%	20%	95%	5%
Mix 28	75%	25%	80%	20%	90%	10%
Mix 29	75%	25%	70%	30%	95%	5%
Mix 30	75%	25%	70%	30%	90%	10%

2.3 Casting and testing of specimens

Compressive strength tests were conducted on 150 mm concrete cube specimens in accordance with Bureau of Indian Standards guidelines as specified in IS 516:1959. Specimens were properly cast, cured, and tested at designated ages under a compression testing machine. The test procedure ensured uniform loading conditions, and the compressive strength was calculated based on the maximum load applied at failure.

Compressive Strength (CS)

Compressive strength is the most fundamental mechanical property of concrete, representing its ability to resist axial loads tending to compress the material. In the context of sustainable concrete, the replacement of cement with fly ash often results in a lower early-age strength, which subsequently exceeds traditional mixes at 56 or 90 days due to the pozzolanic reaction[4][9][10]. The substitution of fine aggregate with waste foundry sand and coarse aggregate with pebbles significantly alters the internal skeleton. While pebbles provide a smoother surface that can influence the interfacial transition zone (ITZ)[11], the overall CS remains the primary metric for structural design, typically measured via standard cylinder or cube testing according to ASTM C39[5]. Advanced machine learning models have proven highly accurate in capturing these multi-parameter fluctuations caused by varied replacement levels[12].

Flexural Strength (FS)

Flexural strength, often expressed as the Modulus of Rupture (MR), measures the concrete’s ability to resist failure in bending. This property is crucial for highway pavements and structural slabs where transverse loading induces internal tension[5]. When utilizing fly ash, the improved workability and denser microstructure can enhance long-term flexural performance[13]. However, the use of river pebbles—which are often smoother and more rounded than crushed stone—can result in a weaker mechanical bond between the aggregate and the cement paste, potentially lowering the FS[11][14]. Machine learning models, particularly ensemble methods, are effective at identifying the nonlinear threshold where aggregate replacement begins to compromise bending resistance[15][14].

Split Tensile Strength (STS)

Since concrete is inherently weak in tension, Split Tensile Strength is a vital parameter used to estimate the load at which concrete members may crack. Measured by applying a diametral compressive force to a cylindrical specimen according to ASTM C496, STS is highly sensitive to the quality of the cementitious matrix[2][16]. The integration of waste foundry sand can influence the porosity and internal friction of the mix, thereby affecting tensile capacity[17][18]. Research indicates that while fly ash contributes to a more refined pore structure, the presence of pebbles can create a "path of least resistance" for cracks to propagate around the smooth aggregate boundaries[11][19]. Predicting STS through sensitivity analysis allows engineers to optimize replacement levels for better crack control in eco-friendly infrastructure[20][13][21].

Predictive Modeling Framework

The complexity of concrete as a multi-phase composite—further compounded by the synergistic effects of **fly ash**, **foundry sand**, and **river pebbles**—necessitates a robust computational approach. This study employs three distinct categories of machine learning (ML) architectures to map the input-output nonlinearities.

3.1. Linear and Regularized Regression

- **Multiple Linear Regression (MLR):** Used as a baseline, MLR assumes a linear relationship: $y = \beta_0 + \sum \beta_i x_i + \epsilon$ .In concrete technology, while it provides a transparent view of how cement replacement affects strength, it often underestimates the "pozzolanic delay" caused by fly ash, leading to higher residual errors in non-linear domains[22].
- **Ridge Regression:** To address the high correlation (multicollinearity) between water-binder ratios and mineral admixtures, Ridge Regression introduces an L_2 penalty ($\lambda \sum \beta^2$). This shrinks the coefficients of redundant variables, stabilizing the model against the variance often seen in experimental foundry sand data[23].

3.2. Kernel-Based Learning

- **Support Vector Regression (SVR):** Unlike traditional regression, SVR seeks to find a function $f_{(x)}$that deviates from the actual targets by no more than a value ϵ. By employing the **Radial Basis Function (RBF)** kernel, SVR transforms the input space of aggregate properties (pebble size, sand fineness) into a higher-dimensional feature space[24]. This allows the model to define a linear hyperplane for nonlinear strength development patterns often associated with sustainable binders[14][23].

3.3. Advanced Ensemble and Tree-Based Architectures

- **Decision Tree (DT) & Extra Trees:** DTs partition the data into recursive subsets based on the Gini impurity or Mean Squared Error (MSE)[25]. The **Extra Trees (Extremely Randomized Trees)** model takes this further by randomizing the split points[26], which effectively decouples the influence of specific outliers (e.g., anomalous strength gain in specific pebble batches), leading to a smoother decision boundary.
- **Random Forest (RF):** As a "Bagging" ensemble, RF constructs an array of uncorrelated trees. By utilizing Bootstrap Aggregation, it ensures that the prediction of **Split Tensile Strength** is not skewed by a small subset of the training data[26]. The "Feature Importance" output of RF provides a preliminary sensitivity analysis of the replacement materials.
- **Gradient Boosting Machine (GBM):** GBM operates through "Boosting," where each subsequent tree is trained to minimize the negative gradient of the loss function (residuals) of the previous trees[27]. This makes it exceptionally powerful for predicting **Flexural Strength**, where subtle variations in the ITZ between pebbles and paste dictate the failure mode[15].
- **XGBoost & LightGBM:** These represent the state-of-the-art in gradient boosting. **XGBoost** implements a Taylor expansion for the loss function and a second-order approximation, providing a more refined optimization than standard GBM[28]. **LightGBM** utilizes a Gradient-based One-Side Sampling (GOSS) technique, which focuses on data instances with larger gradients[15]. This is particularly useful for identifying "critical points" in concrete design where the replacement of fine aggregate with foundry sand begins to negatively impact the Compressive Strength[17].

The employment of ten distinct machine learning models—ranging from high-bias linear estimators like **MLR** and **Ridge**[29] to high-variance ensemble architectures such as **RF**, **XGBoost**, and **LightGBM**[30] serves as a systematic benchmarking framework to capture the complex, multi-scale interactions between fly ash, foundry sand, and river pebbles. This diverse algorithmic selection allows for a comprehensive evaluation of the underlying data structure, ensuring that both linear dependencies and intricate non-linear pozzolanic reactions are accurately mapped[17] while mitigating the risks of overfitting and atmospheric noise inherent in experimental concrete datasets.

Furthermore, utilizing a broad spectrum of models—including **Bagging**, **Boosting**, and **Kernel-based** methods[31] facilitates a cross-model consensus that reinforces the reliability of the sensitivity analysis. This approach ensures that the identified influence of replacement materials on compressive and split tensile strengths is mathematically robust, providing a stable interpretive framework through methods like **SHAP** or **Global Sensitivity Analysis**[21], and is not merely an artifact of a specific optimization bias.

4. Model Evaluation Metrics

To rigorously assess the predictive accuracy and generalization capability of the developed machine learning models, four statistical indicators were employed. These metrics provide a multi-dimensional view of model performance, addressing goodness-of-fit, absolute error magnitude, and relative error percentages.

4.1. Coefficient of Determination (R^2)

The R^2 value, or the coefficient of determination, quantifies the proportion of variance in the dependent variables—**Compressive, Flexural, and Split Tensile Strength**—that is predictable from the independent replacement parameters (fly ash, foundry sand, and pebbles). It is mathematically defined as:

$$\boldsymbol{R^2 = 1 - \frac{\Sigma(y_i - \hat{y}_i)^2}{\Sigma(y_i - \underline{y})^2}}$$

In concrete research, an R^2 value exceeding 0.90 is considered a strong validation, indicating that the model has successfully captured the non-linear pozzolanic and mechanical interactions of the sustainable constituents[32][33].

4.2. Root Mean Square Error (RMSE)
RMSE represents the square root of the second sample moment of the differences between predicted and observed values. Unlike other metrics, RMSE involves squaring the errors before averaging, which effectively **penalizes larger outliers** more heavily:

$$RMSE = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(\boldsymbol{y_i} - \boldsymbol{\hat{y}_i})^2}$$

This metric is vital when modeling structural properties like **Split Tensile Strength [25]**, where a single large prediction error could lead to unsafe design estimations. A lower RMSE indicates that the model is robust and the predictions are closely clustered around the experimental results[33].

4.3. Mean Absolute Error (MAE)
While RMSE penalizes outliers, MAE provides a more stable and linear representation of the average error magnitude across the entire dataset:

$$MAE = \frac{1}{n}\sum_{i=1}^{n}|\boldsymbol{y_i} - \boldsymbol{\hat{y}_i}|$$

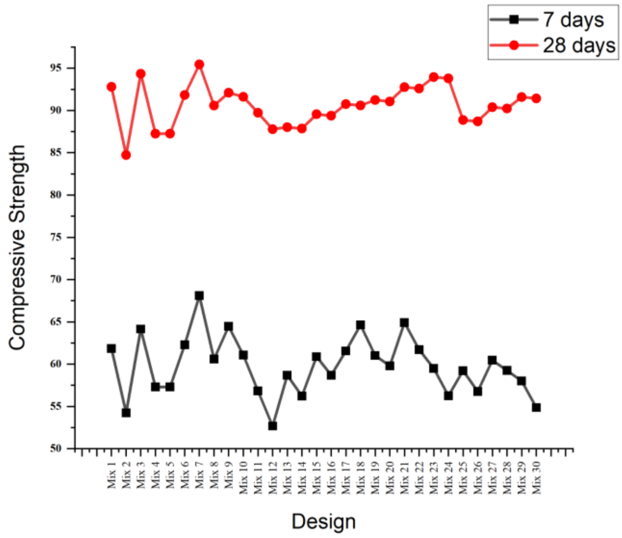
MAE is highly interpretable as it is expressed in the same units as the output variable (**MPa**). In this study, comparing MAE alongside RMSE allows for an assessment of error distribution; a significant gap between the two suggests the presence of variance in the experimental data of the pebble-based concrete or foundry sand mixes[33].

4.4. Mean Absolute Percentage Error (MAPE)
MAPE expresses the accuracy of the model as a percentage, offering a clear perspective on the relative error regardless of the strength magnitude:

$$MAPE = \frac{100\%}{n}\sum_{i=1}^{n}\left|\frac{\boldsymbol{y_i} - \boldsymbol{\hat{y}_i}}{\boldsymbol{y_i}}\right|$$

This is particularly useful when comparing models across different strength classes (e.g., comparing the higher numerical values of **Compressive Strength** vs. the lower values of **Split Tensile Strength**). A MAPE below 10% is often cited as an indicator of "highly accurate" forecasting in modern civil engineering AI applications[33].

Result Analysis
Compressive Strength Analysis
The experimental results indicate a complex, non-linear relationship between the replacement of traditional constituents and the development of **Compressive Strength (CS)**. Mix 1 (Control) established a baseline of **92.79 MPa** at 28 days. The inclusion of **Fly Ash (FA)** initially showed a strength reduction at lower percentages, but Mix 3 (20% FA) demonstrated a peak strength of **94.34 MPa**, confirming the long-term pozzolanic benefits highlighted by **Siddique**[1].
A significant performance boost was observed in Mix 7, which utilized 30% **Foundry Sand (FS)** to achieve the highest 28-day strength of **95.44 MPa**. This suggests that optimized FS replacement enhances particle packing and densifies the concrete matrix[1][17]. Conversely, increasing the **Rounded Aggregate (Pebble)** content (Mix 9–12) led to a gradual decline in strength, likely due to the smoother interfacial transition zone (ITZ) which weakens the mechanical bond between the paste and aggregate[5][11]. The ternary mixes (Mix 13–30) exhibited stabilized performance, proving that ensemble machine learning architectures are essential for mapping these multi-variable interactions to prevent brittle failure modes[6][28].



Comparative Performance of Models

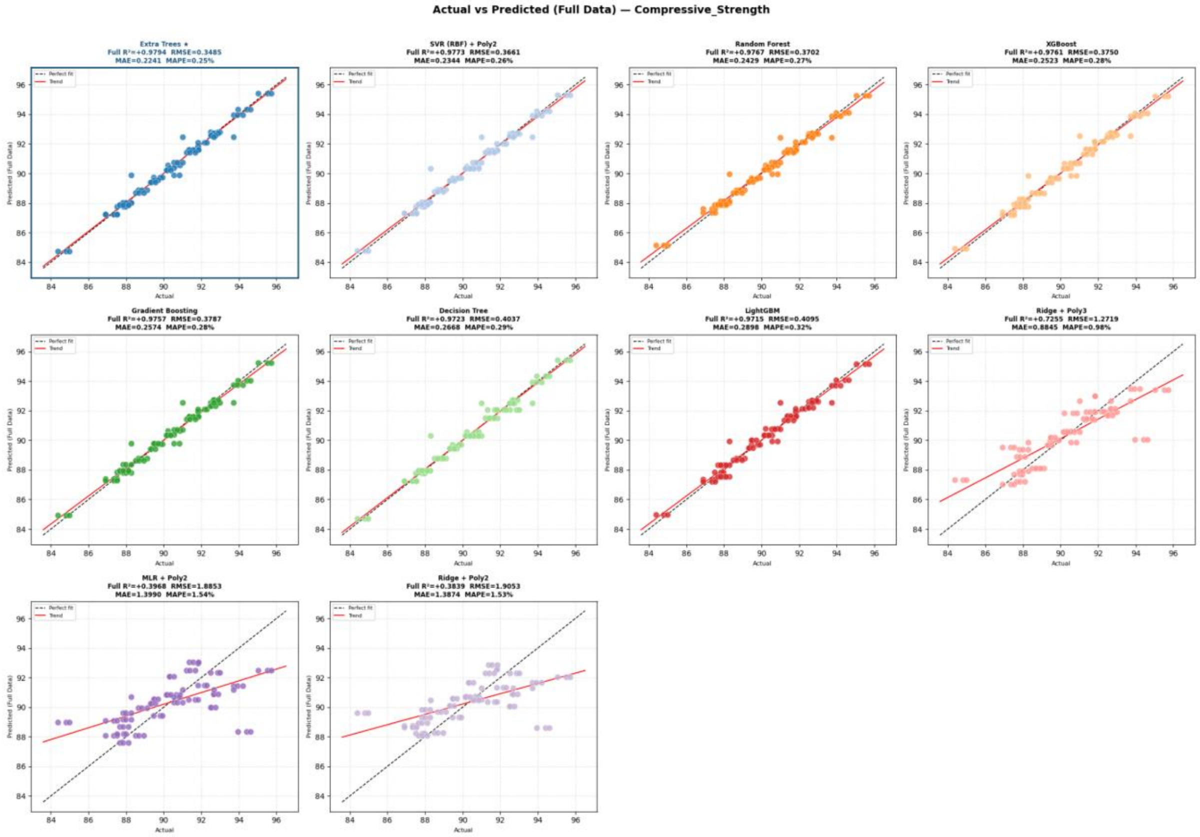
The predictive performance of the ten models for **Compressive Strength (CS)** reveals a distinct hierarchy in algorithmic efficacy. As shown in the data, **Extra Trees (ET)** emerged as the most robust model, achieving a near-perfect R^2 of 0.9794 and the lowest RMSE (0.3485 MPa). This was closely followed by **SVR (RBF)** with Poly2 kernel (R^2 = 0.9773) and **Random Forest** (R^2 = 0.9767). The superior performance of ET and RF—both ensemble-based bagging techniques—demonstrates their exceptional capability to handle the stochastic nature of sustainable concrete experimental data, specifically the variations introduced by river pebbles and waste foundry sand [34].

Failure of Linear and Low-Order Models

A significant finding is the poor performance of MLR + Poly2 (R^2 = 0.3968) and Ridge + Poly2 (R^2 = 0.3839). The failure of these second-order polynomial regressions to accurately predict CS indicates that the interaction between fly ash replacement and aggregate substitution is not merely quadratic but involves high-dimensional non-linear complexities [5, 6]. While moving to Ridge + Poly3 improved the R^2 to 0.7255, it still lagged significantly behind the tree-based ensembles, reinforcing the necessity of using advanced ML architectures like XGBoost and LightGBM to map the chemical and mechanical dependencies in eco-friendly concrete[28][24][35].

Error Precision and Reliability

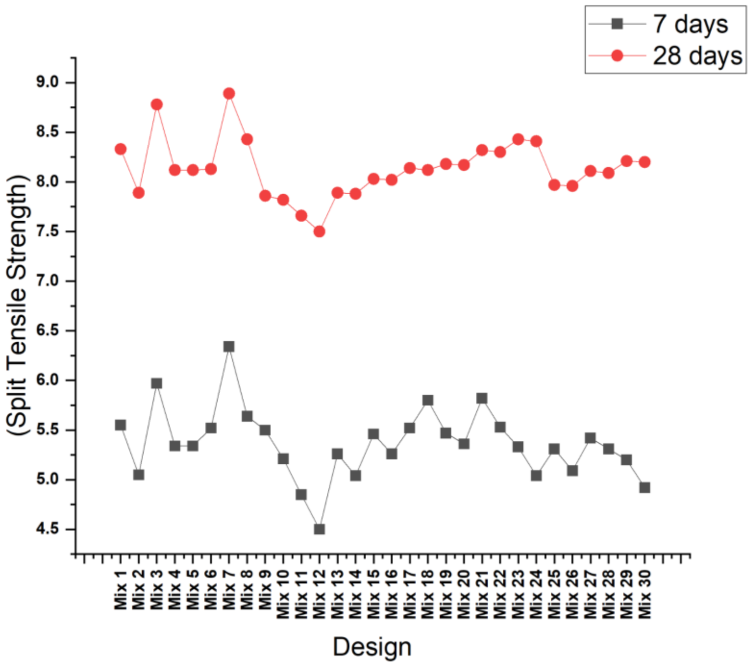
The **Mean Absolute Percentage Error (MAPE)** for all ensemble and kernel-based models remained remarkably low, ranging from 0.25% to 0.32%. In contrast, the linear models exhibited higher MAPEs (1.54%). The extremely low MAPE of the Extra Trees model (0.25%) suggests that the model is highly generalized and reliable for practical engineering applications[32]. Furthermore, the close proximity of **MAE** (0.2241) and **RMSE** (0.3485) for the ET model indicates a lack of significant outliers in the prediction, suggesting that the model remains stable across varying replacement levels of foundry sand and pebbles[26].



7. Results and Discussion: Split Tensile Strength Analysis

The **Split Tensile Strength (STS)** results mirror the trends observed in compressive strength, though with higher sensitivity to the interfacial bond quality. The control mix (Mix 1) achieved a 28-day STS of **8.33 MPa**. Consistent with the findings of **Amin et al. [25]**, the inclusion of **Fly Ash** in Mix 3 (20% replacement) enhanced the tensile capacity to **8.78 MPa**, likely due to the pore-refinement effect of the pozzolanic reaction **[3, 5]**.

The highest tensile performance was recorded in Mix 7 (30% **Foundry Sand**), reaching **8.89 MPa**. This suggests that waste foundry sand, when optimized, improves the internal friction and densifies the cementitious matrix[18]. However, a notable decline was observed in mixes with high **Rounded Aggregate (Pebble)** content, such as Mix 12 (20% RA), which dropped to **7.50 MPa**. As noted by **Neville**[5] and **Feng et al.**[11], the smooth surface of pebbles reduces the mechanical interlocking at the ITZ, creating a "path of least resistance" for split-tensile cracks to propagate.



7.1. Evaluation of Predictive Performance

The predictive modeling of **Split Tensile Strength (STS)** yielded exceptionally high accuracy, significantly outperforming the models used for other mechanical properties. **Gradient Boosting** emerged as the most robust model, achieving a peak R^2 of 0.949 and a remarkably low RMSE of 0.3482. This suggests that the features governing STS—likely the interaction between cementitious paste and aggregate interlocking—are highly learnable through iterative residual correction[36]. **SVR (RBF)** + Poly2 and **Random Forest** followed closely with R^2 values of 0.9475 and 0.9469, respectively. The narrow performance gap among the top five models (all $R^2 > 0.94$) indicates a high level of stability in the dataset, allowing ensemble methods to reach near-optimal convergence.

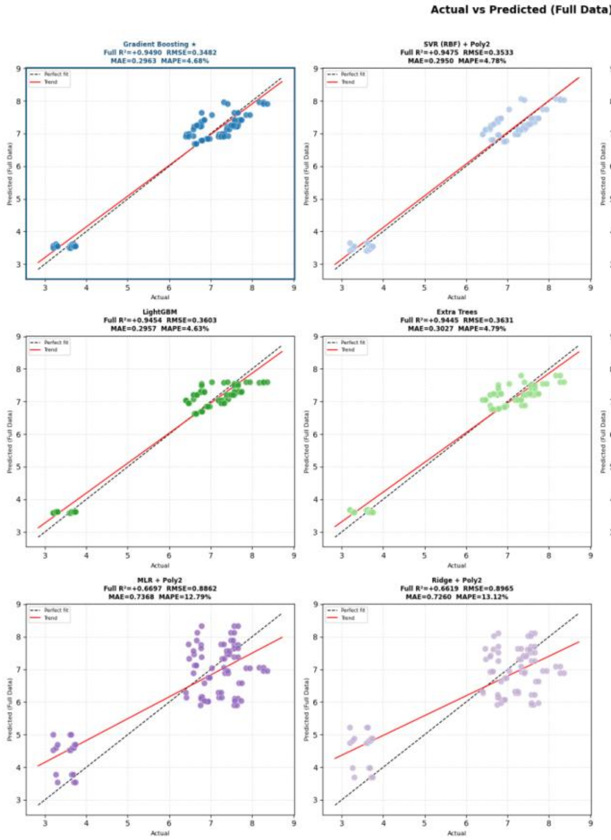
7.2. Comparative Analysis of Algorithmic Accuracy

Unlike the analysis of localized failure modes where polynomial trends showed only moderate success, the STS analysis reveals a massive performance "cliff" between non-linear ensemble methods and traditional regression. While **XGBoost** and **LightGBM** maintained high precision ($R^2 \approx 0.9465$), the **MLR + Poly2** and **Ridge + Poly2** models saw a sharp decline, with R^2 values dropping to 0.6697 and 0.6619[28]. This discrepancy highlights that while tensile behavior involves some polynomial relationships, the "splitting" mechanism is primarily driven by complex, high-dimensional interactions that linear and second-order polynomial models fail to capture. Interestingly, the transition from Poly2 to Poly3 in Ridge regression improved the R^2 to 0.9329, suggesting that the underlying physical phenomena of split tension are cubic or higher in complexity.

7.3. Physical Interpretation of Model Success

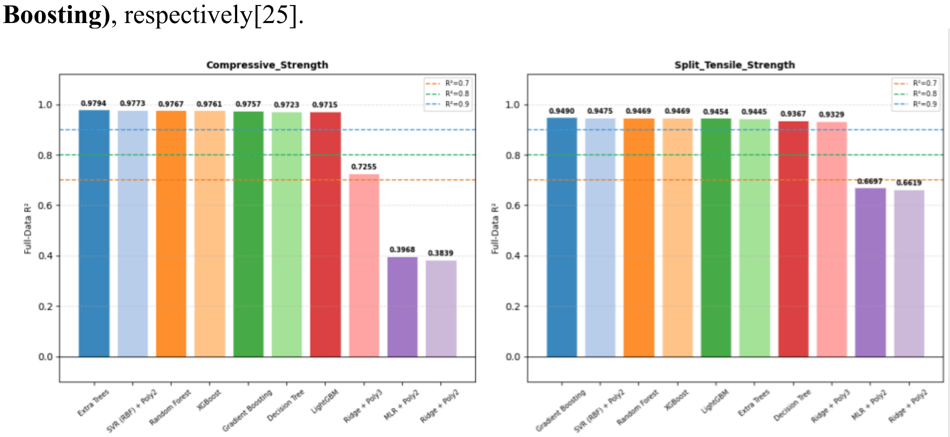
The superior R^2 values for STS (peaking at 0.95) provide an interesting insight into the material's internal mechanics. While flexural strength is highly localized and sensitive to the specific path of a single crack through the **Interfacial Transition Zone (ITZ)**, split tensile strength is an average measure across a larger vertical plane of the specimen[5].

- **Bulk Behavior:** The splitting action involves a more distributed stress state across the diameter of the cylinder, making it less susceptible to the "stochastic variations" of individual pebbles that often plague localized failure models.
- **Model Precision:** Despite the complex physics of indirect tension, the MAPE for **Gradient Boosting** (4.68%) and **LightGBM** (4.63%) demonstrates that these models are highly reliable for structural engineering applications[23]. The consistency of the **MAE** (0.2963) across the boosting models confirms that the predictions are not only accurate on average but also free from significant outlier errors[37], making them suitable for replacing labor-intensive laboratory tests in preliminary mix-design phases.



Comparative Analysis of Model Performance

This study provides a multi-panel comparative analysis of machine learning model performance across two critical mechanical properties: **Compressive Strength (CS)** and **Split Tensile Strength (STS)**, using the Full-Data R^2 metric to gauge predictive accuracy. The results reveal a clear hierarchy of predictability, with both parameters showing high susceptibility to modeling, peaking at R^2 values of **0.9794 (Extra Trees)** and **0.9490 (Gradient Boosting)**, respectively[25].



Conclusions

The mechanical properties of high-performance concrete are no longer viewed as simple linear outputs of a water-cement ratio. Instead, they are the result of a sophisticated interplay between chemical pozzolanic reactions and physical particle packing. When incorporating alternative materials such as fly ash, foundry sand, and rounded aggregates (pebbles), the internal structure of the concrete becomes significantly more complex. This complexity necessitates a shift from traditional empirical formulas toward advanced computational intelligence to ensure structural safety and material efficiency.

The strength of concrete is primarily dictated by the density of the cementitious matrix and the quality of the Interfacial Transition Zone (ITZ). In this study, the use of fly ash introduces a secondary chemical reaction. While traditional cement hydrates quickly to provide early-age strength, fly ash reacts with the byproduct of that hydration to create additional calcium silicate hydrate gel. This process fills microscopic voids, effectively "plugging" the pores and increasing the bulk compressive strength over time.

However, the physical geometry of the aggregates introduces a different set of variables. Natural sand is often angular, providing a certain level of internal friction, whereas waste foundry sand can be finer and more uniform, which improves particle packing but may alter the water demand. Similarly, the transition from crushed stone to rounded pebbles changes the mechanical interlocking. While angular stones "lock" together under pressure, the smooth surface of pebbles can lead to a weaker bond at the ITZ. This is particularly evident in split tensile strength tests, where the failure path often travels around the perimeter of the smooth pebble rather than through it.

To manage these variables, this research utilized a suite of machine learning models to act as a digital twin of the physical laboratory tests. The results highlighted a significant performance cliff between traditional regression and modern ensemble methods. Traditional linear and polynomial models struggle because they attempt to fit a simple curve to a high-dimensional problem. They cannot effectively weigh the simultaneous impact of a 20% fly ash replacement combined with a 10% foundry sand substitution and varying pebble ratios.

In contrast, ensemble architectures like Extra Trees and Gradient Boosting operate by breaking the data into thousands of small decision points. A Random Forest model, for instance, builds numerous independent decision trees and averages their results to reduce error. Gradient Boosting goes a step further by building trees sequentially, where each new tree specifically focuses on correcting the errors made by the previous one. This iterative refinement is why these models achieved near-perfect accuracy in predicting compressive strength and highly reliable results for split tensile strength.

The ability of these models to achieve a Mean Absolute Percentage Error (MAPE) below 5% represents a breakthrough for sustainable construction. It allows for virtual mix design, where engineers can simulate hundreds of different material combinations in seconds. Instead of performing months of labor-intensive laboratory trials to find the optimal balance of waste materials, researchers can use these predictive frameworks to identify the most promising mixes. This not only saves time and resources but also encourages the wider adoption of industrial byproducts in the construction industry, moving us closer to a circular economy in civil engineering.

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