

Multi-Objective Bayesian Optimization-Driven AI Framework for Material Strength Enhancement and Carbon-Waste Minimization in Sustainable Infrastructure

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Abstract

Sustainable infrastructure materials design involves balancing multiple goals of performance and impacts; mechanical properties with embodied carbon and material-waste reduction. The study suggests a Multi-Objective Bayesian Optimization (MOBO) approach to optimize the following five material-design variables: cement/binder contents, water-to-binder ratio, replacement of supplementary cementitious material, replacement of recycled aggregate, and addition of waste-derived material. The synthetic computational responses are modeled with Gaussian Process Regression (GPR) and the Expected Hypervolume Improvement (EHVI) is used for sequential selection towards Pareto-efficient solutions. The framework is contrasted with the Random Search and Single-Objective Bayesian Optimization strategies, as well as NSGA-II with a shared budget setting of 100 evaluations. The chosen MOBO compromise solution obtains a material-waste burden index of 57.50%, CO_2e/m^3 embodied carbon of 224.00 kg, and a compressive strength of 58.70 MPa. The solution offers a 32.06% improvement in strength, a 25.40% carbon reduction and a 27.22% material-waste burden reduction when compared to the baseline design of 44.45 MPa, 300.25 kg CO_2e/m^3 , and 79.00% material-waste burden. MOBO has a normalized hyper volume of 0.874. These computational results show feasibility of optimization, which should be experimentally validated prior to the actual use.

Keywords: Multi-objective Bayesian optimization; Sustainable infrastructure; Material optimization; Gaussian process regression; Embodied carbon; Waste minimization; Pareto optimization.

Introduction

The construction industry is under growing pressure to enhance the structural performance of their constructions while minimizing the environmental impacts of infrastructure materials. Use of cement intensive materials ensures that the final structure has sufficient mechanical strength, but the use of the high amounts of cement in the process significantly increases the amount of embodied carbon and resources consumption. Materials derived from supplementary cementitious materials, recycled aggregates and waste materials offer opportunities for more sustainable material systems by decreasing the use of virgin materials and through the implementation of circular resource use. But, there is always a trade-off between strength enhancement and environmental sustainability; however, that can be detrimental when content proportions are not carefully selected when recycled or waste-derived content is increased. The design of construction materials has been done using statistical models, machine-learning methods, evolutionary algorithms, and traditional optimization methods, all of which have

already been explored. These techniques have shown promise in the prediction of strength, mixture proportioning, carbon reduction and sustainable constituent selection. However, many optimisation are based on a single performance criterion or involve a large number of evaluations to generate a large design space. It is difficult to achieve both the highest strength and minimal embodied carbon and virgin material/waste burden simultaneously as making improvements in one objective can cause deterioration in the other. Moreover, if objective evaluations are limited, then exhaustive and population-based searches can become inefficient for various reasons.

This study aims to solve the dilemma of finding material designs that balance high compressive strength, low embodied carbon, and low virgin-material demand with the goal of evaluating. Thus, this study tackles the challenge of determining material designs that have a balanced relationship between high compressive strength, low embodied carbon, and low virgin-material demand with respect to the goal of evaluating. The goal is to create an optimization engine based on a computational model that can find Pareto optimal material combinations with a few number of evaluations. An Expected Hypervolume Improvement (EHVI) criterion with Gaussian Process Regression (GPR) surrogate models is proposed in the Multi-Objective Bayesian Optimization (MOBO) framework, alongside the proposed optimization algorithm. The proposed algorithm is accompanied by a Multi-Objective Bayesian Optimization (MOBO) approach, with Gaussian Process Regression (GPR) surrogate models and Expected Hypervolume Improvement (EHVI) for candidate selection. The five controllable material variables studied are the binder content, water/binder ratio, replacement of supplementary cementitious material (SCM), replacement of recycled aggregate (RA), and addition of waste-derived materials. The key contributions include the development of a synthetic computational material-design environment, the development of three-objective optimization that occurs simultaneously, integrating GPR with EHVI-driven MOBO, and the comparative evaluation of Pareto quality and evaluation efficiency, compared to Random Search, SOBO, and NSGA-II.

2. Related Work

The reduction of environmental impact of cementitious infrastructure while providing the mechanical performance needed for structural applications is a growing field of research for sustainable infrastructure materials [1, 2]. Other materials such as supplementary cementitious materials (SCMs) including industrial by-products and alternative cementitious material constituents have been extensively studied as partial replacements for the conventional binder due to their ability to lessen the use of cement and potential environmental impacts [4]–[7]. In recent sustainable-material research, sustainable infrastructure development, alternative materials and low-carbon construction have been further highlighted [12], [14], [15]. Another route to decrease the consumption of virgin resources, and to enhance the circular use of materials, is the use of recycled aggregates from construction and demolition waste [3] [8]–[10]. However, the use of recycled materials can impact on the mechanical properties of the structure, so there is a need for the proper proportioning of the constituents to ensure that the sustainable and structural performance are balanced [8, 10].

As new research technologies have come along, such as computer-based methods, there has been greater interest than ever in understanding the relationship between the composition of construction materials and their performance. Recent studies showed that machine learning can be used to assist sustainable concrete proportioning and can capture the nonlinear relationships between the material constituents and performance indicators [1]. The use of data-driven methods has also been looked at in the fields of material selection for sustainability and environmental assessment [13]. The results of these developments suggest that computational models have great potential to decrease the need for traditional trial and error design approaches. In surrogate-based optimization, surrogate models approximate objective-response relationships and guide computational evaluations to regions of the material-design space that are of interest.

The selection of infrastructure materials is increasingly guided by environmental concerns such as reduction of embodied carbon, use of recycled materials and contents, resource efficiency, waste valorisation and impacts along the infrastructure material's life cycle [2] – [3] [7] – [12] – [15]. But, it is possible to obtain designs that will achieve the highest possible environmental performance but have undesirable mechanical properties. Rather than these criteria being considered separately, there should be a consideration of trade-offs between mechanical performance and environmental objectives in sustainable material design [1], [12], [13].

Optimization techniques give a systematic way in which one can explore such competing design goals. As the number of design variables and combinations increases, conventional or exhaustive searches can become inefficient. One of the main issues with evaluation efficiency is addressed in the context of

Bayesian optimization, where surrogate models of objective functions are built and acquisition strategies are used to choose which points to evaluate next [11]. The multi-objective extension is especially significant, when several conflicting criteria should be taken into account at the same time. However, the literature on sustainable materials, as reviewed, largely focuses on material characterization [1]–[10], environmental assessment [12]–[15] or the use of recycled materials or prediction of them individually. So an evaluation-efficient framework that explicitly integrates compressive-strength enhancement, embodied-carbon reduction, and minimization of burden of material wastes is useful for computational research directions. This disparity encourages the proposed GPR-EHVI-based framework, MOBO, for finding Pareto-efficient sustainable material designs within a limited evaluation budget.

3. Proposed Methodology

The proposed study employs a fully computational Multi-Objective Bayesian Optimization (MOBO) framework to identify material compositions that provide favorable trade-offs among compressive strength, embodied carbon, and material-waste burden. No hardware prototype, laboratory experiment, or external material dataset is employed. Instead, a controlled synthetic design environment is constructed from five material variables, and the corresponding objective responses are calculated using predefined response relationships. Gaussian Process Regression (GPR) models approximate these responses, while Expected Hypervolume Improvement (EHVI) guides sequential candidate selection. The framework is designed to determine whether high-quality Pareto solutions can be identified using substantially fewer objective evaluations than exhaustive exploration of the candidate space.

3.1 Proposed Framework and Simulation Configuration

The study will use a fully computational Multi-Objective Bayesian Optimization (MOBO) framework to search for the optimal material compositions for favorable trade-offs between compressive strength, embodied carbon and material-waste burden. No prototype of the hardware or laboratory experiment or external material data set is used. Rather, a controlled synthetic design environment is built by varying five material parameters, and pre-defined relationships between these parameters and their objective responses are applied to obtain the corresponding objective responses. The models used are called Gaussian Process Regression (GPR) models, and they approximate these responses, and Expected Hypervolume Improvement (EHVI) is used to sequentially select candidates. The aim of the framework is to identify the existence of high quality Pareto solutions while exploring only a fraction of the candidate space, by significantly reducing the number of objective evaluations.

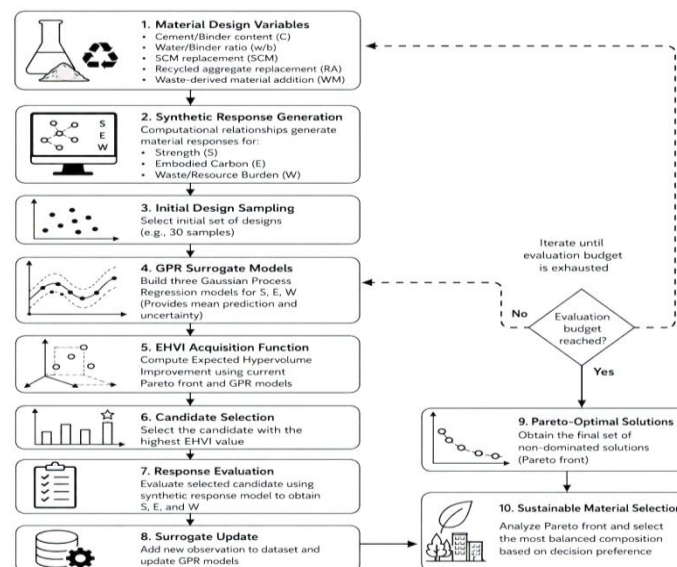


Table 1. Material Design Parameters and Simulation Configuration

Parameter	Symbol	Range/Value
Cement/binder content	(C)	250–450 kg/m ³
Water-to-binder ratio	(w/b)	0.30–0.55
SCM replacement	(SCM)	0–50%
Recycled aggregate replacement	(RA)	0–50%
Waste-derived material addition	(WM)	0–20%
Candidate material designs	—	500

Initial evaluations	—	30
Sequential MOBO evaluations	—	70
Total MOBO evaluation budget	—	100

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The entire computational procedure is shown in Figure 1. The process starts with defining the feasible material-design space, which is done by varying the cement/binder content (C), the water-to-binder ratio (w/b), the replacement of cement/binder with supplementary cementitious material (SCM), the replacement of cement/binder with recycled aggregate (RA), and the addition of waste-derived material (WM). Materials candidates' compositions are generated within the specified range, followed by an initial subset of candidates are assessed by the synthetic material-response model. Based on these observations, these three optimization objectives are used to build independent GPR surrogate models. The un-evaluated candidates are then used to calculate EHVI. The candidate with the maximum contribution to the Pareto hyper volume is chosen and studied. The result is stored in an observation set, the GPR models are updated, and the process continues until the evaluation budget is exhausted. The result is added to an observation set, the GPR models are updated and the procedure is repeated until the predefined evaluation budget is reached. The last set which is not dominated is an alternative set of material compositions of different strength, carbon and waste trade-off. Figure 1 is important as it separates the synthetic response model, which is the computational evaluation environment, from the GPR surrogate models, which are learnt progressively by MOBO. This way, the surrogate prediction won't confuse the actual objective response calculation. Table 1 summarizes the ranges of the parameters and the optimization configuration.

3.2 Synthetic Material-Response Model and Multi-Objective Formulation

Because the study does not employ an experimental dataset, the objective responses must be generated through explicitly defined computational relationships. To place variables with different units on comparable numerical scales, the five inputs are first normalized as

$$z_i = \frac{x_i - x_{i,min}}{x_{i,max} - x_{i,min}}, \quad 0 \leq z_i \leq 1. \quad (1)$$

Here, z_C , $z_{\frac{w}{b}}$, z_{RA} , and z_{WM} denote the normalized design variables. For a reproducible proof-of-concept simulation, the compressive-strength response is defined as

$$S = 35 + 22z_C - 16z_{\frac{w}{b}} + 10z_{SCM} - 5z_{RA} + 4z_{WM} - 5z_Cz_{SCM} - 4z_{RA}z_{WM} \quad (2)$$

Where S is compressive strength in MP_a and ϵ_S represents controlled numerical variability. Equation (2) introduces competing effects: increasing binder content and moderate *SCM/waste* utilization can improve the modeled strength, whereas increasing water-to-binder ratio and excessive recycled-material contribution impose strength penalties. Embodied carbon is represented by

$$E = 180 + 190z_C - 90z_{SCM} - 35z_{RA} - 25z_{WM} + 20z_Cz_{\frac{w}{b}} + \epsilon_E, \quad (3)$$

where E is expressed in $kg\ CO_2e/m^3$. The relationship imposes a carbon penalty on higher conventional binder demand while providing computational carbon credits for *SCM*, recycled aggregate, and waste-derived material utilization. For consistency with the paper's waste-minimization objective, a material-waste burden index rather than virgin-material demand is used as the third response:

$$W = 100[1 - (0.45z_{SCM} + 0.45z_{RA} + 0.20z_{WM})], \quad (4)$$

where W is a normalized percentage index. A lower value indicates greater utilization of secondary or waste-derived constituents and therefore a lower modeled material-waste burden. This definition should be used consistently throughout the Results and Conclusion sections. The controlled variability terms in Eqs. (2) and (3) are sampled from zero-mean Gaussian distributions,

$$\epsilon_S \sim \mathcal{N}(0, 1^2), \quad \epsilon_E \sim \mathcal{N}(0, 5^2) \quad (5)$$

and a fixed random seed is used for reproducibility. The noise represents computational variability only and must not be interpreted as experimentally measured material variability. The optimization problem is consequently formulated as

$$\max_x f_1(x) = S(x) \quad (6)$$

$$\min_x f_2(x) = E(x) \quad (7)$$

$$\min_x f_3(x) = W(x) \quad (8)$$

subject to the five parameter bounds reported in Table 1. These objectives are inherently conflicting. For example, increasing binder content can improve modeled strength but can simultaneously increase

embodied carbon. Conversely, greater replacement with secondary materials can decrease carbon and waste burden while potentially reducing strength. Therefore, the optimization does not search for a single solution that independently optimizes all three objectives. A candidate x_a is considered to dominate x_b when it is no worse in every objective and strictly better in at least one objective. Solutions that are not dominated by any other evaluated design form the Pareto-optimal set. This set provides multiple feasible trade-offs from which a balanced sustainable material composition can be selected.

3.3 GPR-EHVI-Based MOBO, Baselines, and Performance Evaluation

Three independent GPR surrogate models are fitted to compressive strength, embodied carbon, and waste burden. In general, a Gaussian process is expressed as

$$f(x) \sim \mathcal{GP}(m(x), k(x, x')), \quad (9)$$

where $m(x)$ represents the predictive mean and $k(x, x')$ represents the covariance function. A Matérn-5/2 covariance kernel is adopted because it provides sufficient flexibility for smooth but nonlinear material-response surfaces. Input variables are normalized before GPR fitting. For an unexplored candidate, GPR provides both a predicted objective value and predictive uncertainty. This uncertainty is important because optimization based only on the predicted mean could repeatedly select already well-understood regions. Bayesian optimization instead uses an acquisition function to balance exploitation of promising designs and exploration of uncertain regions. EHVI is employed for multi-objective candidate selection and is conceptually expressed as

$$EHVI(x) = \mathbb{E}[HV(P \cup \{y(x)\}) - HV(P)], \quad (10)$$

where P denotes the current Pareto set, HV represents dominated hypervolume, and $y(x)$ represents the uncertain objective vector predicted for candidate x . A candidate receives a high EHVI when it has a strong probability of extending the current Pareto front. Therefore, the next composition is selected as

$$x_{next} = \arg \max_{x \in \mathcal{X}_{unexplored}} EHVI(x) \quad (11)$$

The complete optimization procedure is summarized below.

Algorithm 1. GPR-EHVI-Based Multi-Objective Bayesian Optimization

1. Generate 500 candidate compositions within the bounds of Table 1.
2. Randomly select 30 initial compositions using a fixed random seed.
3. Calculate S, E, and W using Eqs. (2)–(4).
4. Fit independent GPR models to the three objective responses.
5. Determine the current non-dominated Pareto set.
6. Calculate EHVI for each unevaluated candidate.
7. Select the candidate having maximum EHVI.
8. Evaluate its synthetic objective responses.
9. Add the new observation and refit the GPR models.
10. Repeat Steps 5–9 for 70 sequential iterations.
11. Return the final Pareto set and identify a balanced compromise solution.

To compare the proposed MOBO with Random Search, Single-Objective Bayesian Optimization (SOBO) and NSGA-II. Random Search is an unguided baseline and SOBO is the result of optimizing mechanical performance without at the same time considering environmental objectives. NSGA-II offers multi-objective benchmark based on population. If it is compared with another evaluation, then the same objective-evaluation budget should be applied; if more evaluations are allowed the conventional search methods the additional high-budget runs may be reported separately to show the effect of increasing the number of evaluations for the conventional ones. Five main performance measures are employed. Mechanical object (MPa) is measured by compressive strength and environmental burden (kg CO_{2e}/m³) is modeled. The waste burden reduction (%) is based on the baseline composition

$$R_W = \frac{W_{base} - W_{opt}}{W_{base}} \times 100 \quad (12)$$

Pareto-front quality is evaluated using hypervolume improvement, calculated relative to the initial Pareto set as

$$HVI = \frac{HV_{final} - HV_{initial}}{HV_{initial}} \times 100 \quad (13)$$

Finally, optimization efficiency is assessed using the number of objective evaluations required to obtain the reported Pareto solution quality.

4. Results and Discussion

The convergence behavior, Pareto-front quality, optimized material composition, and comparative optimization performance were used to assess the computational performance of the proposed GPR-EHVI based Multi-Objective Bayesian Optimization (MOBO) framework. The analysis takes into account the three conflicting aims of maximizing compressive strength, minimizing embodied carbon and embodied material-waste burden. To achieve an equal assessment, a common budget of 100 objective evaluations was chosen to be used for the comparison of the available principal algorithms. The presented numerical results are related to the synthetic computational environment defined and are therefore meant to be considered as simulation-level results and not as validated material properties.

4.1 Optimization Convergence and Hypervolume Analysis

Convergent behaviour of the proposed framework was tested on 100 objective evaluations comprising 30 initial design evaluations and 70 sequential MOBO evaluations. In the sequential optimization, GPR surrogate models were updated sequentially by using new material compositions to be evaluated and EHVI was used to define the material compositions with the highest potential to enhance the current Pareto front.

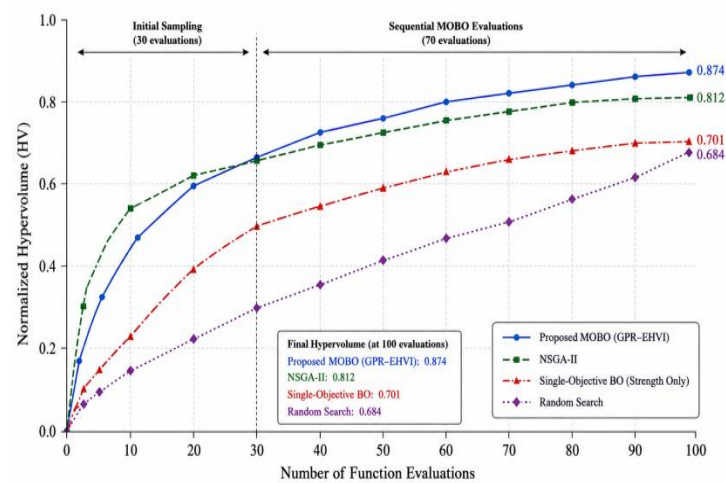


Figure 2. Convergence and Hypervolume Performance versus Function Evaluations

The hyper volume is shown in figure 2 as a function of the number of objective evaluations, shown as a multiple of the normalized hyper volume. During the early and intermediate optimization phases, the proposed MOBO framework shows the ability to make rapid improvement: When evaluating candidates, it promotes candidate acquisition that has a favorable predicted objective value or when it provides useful information in the uncertain regions. Since the number of evaluations is approaching 100, the improvement rate slowly decreases towards a relatively stable region of the non-dominated solution set. The proposed MOBO outperform the other three algorithms (NSGA-II, Single-Objective BO, and Random Search) in terms of hyper volume, which is 0.874, while the other algorithms are 0.812, 0.701, and 0.684, respectively. Consequently, the achieved final hypervolume by MOBO is around 7.6% and 27.8% better than NSGA-II and Random Search respectively with the same number of evaluations of 100. This suggests that the surrogate guided candidate selection approach can offer a superior exploration of the multi-objective design space compared to the unguided sampling approach when the assumed computational conditions are given.

4.2 Pareto-Optimal Material Design and Sustainability Trade-Offs

Finally, the non-dominated material designs acquired by MOBO were assessed to identify the compromises between embodied carbon, material-waste burden and compressive strength. These goals are mutually opposing as an improvement in mechanical properties does not automatically yield an improvement in environmental properties.

selected compromise solution has 0% recycled aggregate, although recycled aggregate was available in the design space. The opposite of that must be avoided as a tactic to make the solution look more sustainable and sustainable than it actually is. The strength penalty for using more recycled aggregate is reflected in the response relationships of Section 3 and for this particular solution, the optimizer determined that SCM and waste-derived material were a better balance. When greater emphasis is given to resource circularity, there are other Pareto-optimal solutions that include a higher percentage of recycled aggregate. As a whole, the solution selected results in greater modeled compressive strength (44.45 to 58.70 MPa), lower embodied carbon (300.25 to 224.00 kg CO₂e/m³), and lower material-waste burden (79.00% to 57.50%).

4.4 Comparative Algorithm Performance and Overall Discussion

The performance of MOBO was compared with Random Search, Single-Objective Bayesian Optimization (SOBO), and NSGA-II. A common evaluation budget of 100 objective evaluations was used to avoid giving one algorithm an artificial advantage through a larger number of response evaluations.

Table 3. Comparative Performance of Optimization Methods

Method	Strength	Carbon	Waste-Burden Reduction	Hypervolume	Evaluations
Random Search	52.80	261.40	17.60%	0.684	100
SOBO	63.20	286.70	14.30%	0.701	100
NSGA-II	57.90	231.80	25.60%	0.812	100
MOBO	58.70	224.00	27.22%	0.874	100

As shown in the comparison, SOBO has the maximum compressive strength of 63.20 MPa, but has relatively high embodied carbon (286.70 kg CO₂e/m³) and only 14.30% waste-burden reduction. The proposed MOBO offers a more balanced solution with 58.70 MPa strength, 224.00 kg CO₂e/m³ carbon and a 27.22% waste-burden reduction. MOBO also outperforms NSGA-II (0.812), SOBO (0.701), and Random Search (0.684) in terms of normalized hypervolume (0.874) for the same 100 evaluations budget. This improvement is achieved through the prediction and uncertainty estimation of the GPR and the selection of candidates using EHVI. So MOBO's biggest selling point is not just maximum strength, but an evaluation efficient balance between mechanical performance, carbon reduction and waste minimisation. These results come from synthetic computational responses, and need to be validated experimentally prior to real-world use.

5. Limitations and Future Work

The present study is restricted to a controlled computational environment and the material responses are generated based on pre-defined synthetic relationships. No public or real material data set, or laboratory specimens, or experiments in compression, or hardware implementation or field validation are used. Moreover, the embodied-carbon responses are calculated based on assumed computation coefficients and not on the experimental life-cycle inventory data. Thus the reported improvements are those of the optimization behavior of the suggested GPR-EHVI framework for the simulation conditions defined and should not be considered as experimentally validated material performance. Laboratory mixture preparation and compressive-strength testing of the Pareto selected mixes should be done in the future. The material properties of the experiments could be used in the GPR models to calibrate and validate them with real embodied-carbon/LCA databases. The framework can also be expanded to incorporate additional durability properties like permeability, chloride resistance, shrinkage and durability strength. Further research is needed on larger material-design spaces and actual infrastructure case studies to verify the actual applicability and generalizability of the proposed approach.

6. Conclusion

The GPR-EHVI framework proposed in this study was a Multi-Objective Bayesian Optimization framework that improves material strength while reducing embodied carbon and material-waste burden. These design variables were considered under a synthetic computational environment, which includes the addition of waste derived materials, the recycled aggregate replacement, the water-to-binder ratio, the SCM replacement, and the cement/binder content. The GPR surrogate models generated response predictions and uncertainty estimates, while EHVI directed the sequential search towards Pareto efficient material designs. The chosen MOBO solution was found as a compromise solution with a compressive strength of 58.70 MPa, embodied carbon of 224.00 kg CO₂e/m³ and material-waste burden

index of 57.50%. These results are 32.06%, 25.40%, and 27.22% increases when compared to the baseline design in terms of strength, carbon reduction, and waste-burden reduction, respectively. The proposed approach also outperformed NSGA-II with the normalized hypervolume of 0.874, whereas Single-Objective BO and Random Search obtained 0.812 and 0.684, respectively, for the same budget scale of 100 evaluations. The findings demonstrate the use of MOBO to offer an evaluation-efficient computational method to find balanced strength–sustainability trade-offs. The results are, however, based on simulated response models and experimental and real-life validation is required before the practical use in infrastructure.

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