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Automating life cycle assessment for additive manufacturing with machine learning: Framework design, dataset buildup, and a case study

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ABSTRACT

Additive Manufacturing (AM) has been regarded as a technology with disruptive potential, offering the possibility of substantial reductions in the environmental footprint. The predominant approach to quantitatively evaluate AM's environmental impacts relies heavily on the knowledge-intensive and time-consuming Life Cycle Assessment (LCA) methodology. To enable a faster design iteration cycle and alleviate the knowledge requirements of LCA modeling, the availability of an automated LCA tool could mark a remarkable leap forward in further enhancing AM's environmental performance. An emerging solution to achieve this goal is the combination of Machine Learning (ML) with LCA, the effectiveness of which has been initially demonstrated outside the AM domain. To explore the feasibility of predictive LCA for AM, this paper proposes a novel data-driven framework that integrates ML, product-process codesign, and LCA to support the environmental impact prediction of AM. The efficacy of the proposed methodology is demonstrated by taking the Fused Filament Fabrication (FFF) process as a case study. This work introduces three main contributions to the research community. First, a training dataset comprising 200 data entries, where each entry encompasses 5 design features, 7 process features, and 18 environmental impact categories is constructed. Second, through a two-stage process involving correlation analysis and an ML preliminary study, the initial 12 design-process parameters are refined to 7 key influential features. Lastly, the refined set of features and 7 different ML algorithms are employed to develop a data-driven LCA (DD-LCA) model for the FFF process. Notably, the Extreme Gradient Boosting (XGBoost) and Multi-Layer Perceptron (MLP) algorithms demonstrate good performance with a prediction accuracy of 98% and a root mean square error (RMSE) of 0.029. The developed model exhibits good generalizability when tested on new data. The paper concludes by addressing its limitations and outlining future research work.

1. Introduction

Additive Manufacturing (AM) stands out as a promising and innovative technology to fabricate goods with green characteristics [1–3]. The boundless range of intricacy, adaptability, and environmentally friendly attributes presented by this technology grants the possibility to incorporate 3D printers as an essential component of the contemporary manufacturing era [4]. AM has been recognized as having the potential to offer various environmental sustainability benefits. One of these advantages is the production of minimal waste during manufacturing, thanks to its additive nature. AM also enables the optimization of geometries and the creation of lightweight components, resulting in reduced material consumption during manufacturing and lower energy consumption during use. Additionally, AM contributes to decreased transportation requirements within the supply chain and minimizes inventory waste by enabling the on-demand production of spare parts [5]. Life cycle analyses have demonstrated that the adoption of AM could lead to substantial cost savings in the production of goods. By 2025, the potential savings could range from $113 billion to $370 billion. These savings would be achieved through reductions in material inputs and handling, as well as the streamlining of supply chains resulting in shorter transportation distances and lower associated costs [1].

While AM applications are quickly transitioning from rapid prototyping to the production of end-use products, the environmental impacts associated with this technology, as well as the corresponding material flows, remain an area of ongoing exploration and investigation. In an attempt to gain a better understanding of the consequences of such impacts, qualitative studies examining the social [6], economic [7], and

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environmental [8] aspects of sustainability in AM have been reported in the literature. However, qualitative research on AM's sustainability cannot provide enough insights to fully understand its sustainability potential. On the other hand, most of the existing quantitative studies on the environmental impact assessment of AM rely on the classical Life Cycle Assessment (LCA) methodology and its applications [9–11] to assess its environmental performance. However, many practitioners and designers find it challenging to utilize LCA tools [12,13]. This is primarily due to the perceived high costs associated with conducting LCA, the need for subjective assessments of environmental priorities, and the requirement for extensive knowledge and expertise to carry out the analysis effectively [14]. Such a data-intensive procedure can be inefficient in the early process design stages where a significant amount of essential background and foreground inventory data is yet to be obtained [13]. Further, current studies on assessing the environmental performance of AM show a disconnection between design and process parameters. This is because the majority of these studies are either design or process-oriented [15–17]. Even existing studies on assessing the environmental impacts of AM through the concept of product-process co-design [18,19] have utilized specific AM design and process parameters without justifying their selection of influential parameters/strategies (AM design and process parameters/strategies that pose significant impacts on AM's environmental performance). Consequently, the role of AM in facilitating the transition toward a more environmentally benign production remains ambiguous. As such, the research community demands better tools to accurately assess the environmental impacts of AM with reduced knowledge requirements.

Today, there is an increasing trend and dedicated efforts toward utilizing Machine Learning (ML) to estimate LCA data. The integration of ML with LCA has demonstrated its efficacy in predicting and significantly reducing the environmental impacts of buildings [20,21] and estimating the life cycle impact of chemicals [22]. Further, ML has been successfully employed in estimating unit process data [23], carbon emissions [12], quantifying greenhouse gas emissions [24], evaluating LCA metrics of bio-based and biorefinery processes [13], and determining chemicals characterization factors [25]. Although ML has been successfully adopted in various AM applications (e.g., fabrication planning [26], quality control [27], process parameters optimization [28]), there is a paucity in the literature regarding ML-assisted LCA for AM.

Accordingly, the goal of this research is to develop an automated tool to predict the environmental impacts of the AM process. The primary objective of this tool is to provide decision-makers with expeditious yet accurate automated decision support to facilitate their comprehension and mitigation of these impacts. To achieve this ultimate objective, this study first introduces a novel data-driven life cycle assessment (DD-LCA) framework for AM. The framework follows the complete workflow of the AM process, encompassing initial design stages to the production of the final printed part. By considering both product design and process parameters, the framework offers a comprehensive assessment of the environmental impacts of AM. The efficacy of the proposed framework is then demonstrated by taking the Fused Filament Fabrication (FFF) process as a case study. Following that, a training dataset comprising 200 data points is constructed. Next, correlation analysis and an ML preliminary study are employed to spot correlated features and identify key influential parameters. Thereafter, seven different ML algorithms are constructed and compared. Subsequently, the generalizability of the constructed model is tested on previously unseen data. Finally, the developed model is utilized to promptly identify environmental "hotspots", offering guidance to designers and decision-makers by recommending areas where adjustments and improvements can yield the greatest ecological advantages. The developed DD-LCA tool is expected to provide instant sustainability evaluation guidance, allowing designers to make sustainability and ecological-related decisions in the early stage of design and production. The implementation of such an automated tool should also efficiently substitute the current "fix it later" approach which is based on limited potential sustainability benefits due to the late consideration of sustainability within the design process. Thus, the DD-LCA tool is expected to save cost, time, and experimental efforts.

The remainder of this paper is structured as follows. Section 2 sheds the light on the various LCA-based methodologies employed to evaluate the environmental impacts of AM. This is subsequently followed by summarizing the various AM's environmental sustainability influential parameters and strategies. Additionally, this section introduces the various applications of ML in sustainable manufacturing. This section concludes by providing an overview of the various studies that have integrated ML with LCA to develop automated tools to assess the environmental impacts of applications outside the AM domain. Section 3 then introduces the proposed DD-LCA framework. Section 4 explores the construction of the DD-LCA model including the process of data collection, pre-processing, the various ML algorithms employed, and feature selection evaluation. Section 5 delves into the performance evaluation of the DD-LCA model, presenting the evaluation metrics in addition to result analysis and discussions. This is then followed by discussing the model generalizability on unseen data and the identification of hotspots. Finally, Section 6 presents some concluding remarks, limitations, and future research directions.

2. State of the art

In this section, our exploration commences by examining the quantitative environmental impact assessment of AM through the lens of LCA methodologies. Then, we shift our focus on identifying the various influential parameters and strategies of AM's environmental sustainability. Furthermore, we extend our exploration to encompass the transformative potential of ML in sustainable manufacturing. Finally, we explore the use of ML in LCA for applications beyond AM.

2.1. LCA-based quantitative environmental impact assessment of AM

The majority of the existing quantitative research on the environmental evaluation of AM revolves around the utilization of the classical LCA methodology. These studies can be classified into three categories: those focused on modeling the environmental impacts of individual AM processes [18,29,30], and those comparing the environmental effects between different AM technologies [31–33] or between AM and conventional manufacturing (CM) approaches [9–11].

Studies falling into the category of unit AM process modeling have primarily concentrated on the production phase within the AM's life cycle. These studies have explored various materials and AM technologies. Further, these studies vary in the inclusion of factors such as embodied energy in machines and auxiliary tools, raw material production, and post-processing in their analyses. A wide range of AM processes, such as Selective Laser Sintering (SLS) [18,34], Selective Laser Melting (SLM) [35], Fused Filament Fabrication/Fused Deposition Modeling (FFF/FDM) [36], Binder Jetting [30,37], and Stereolithography (SLA) [38] have been examined in these reported studies. A prevailing consensus among the majority of these studies is that energy and material consumption are the primary contributors to the environmental impacts associated with AM.

Studies under the second category have focused on comparing the environmental impacts of different AM technologies. The scope of the LCA considered, such as Cradle-to-Grave or Cradle-to-Gate, as well as the specific resources analyzed (e.g., materials, energy), vary among these studies. For example, some investigations have focused solely on comparing the energy consumption of metal-based technologies and polymeric AM processes [39], FFF and Binder Jetting [40] or between metal wire-based and powder-based AM technologies [41]. Li et al. [32] conducted a comparative study on the environmental impacts of polymeric FFF/FDM, SLA, and Polyjet AM techniques. Their findings revealed that FFF/FDM parts exhibited the lowest environmental impact, while parts fabricated through PolyJet exhibited the highest environmental impact. This disparity can be attributed to the lower

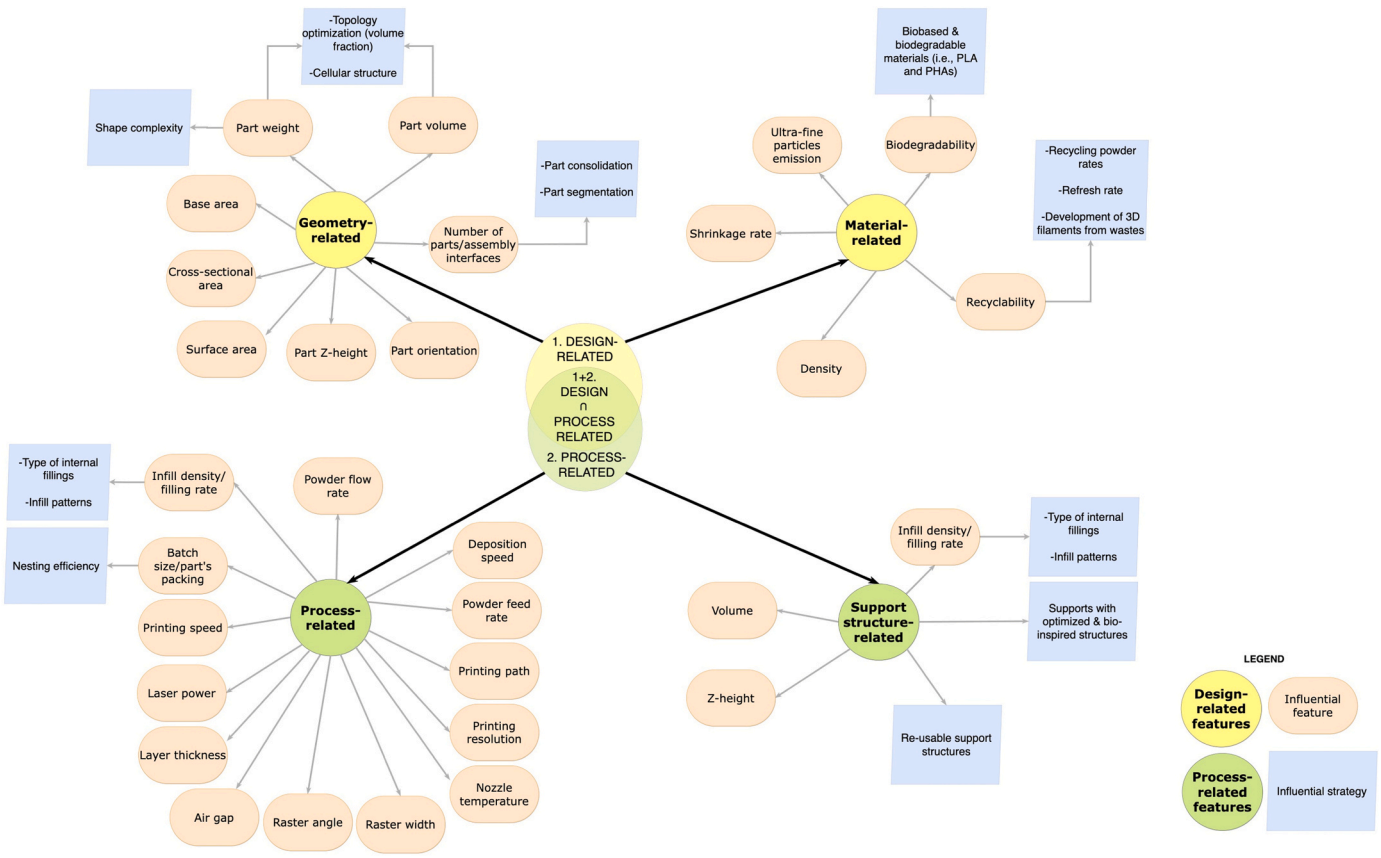

Fig. 1. Overview of the different influential parameters and strategies impacting the environmental sustainability of AM.

process energy consumption in FFF/FDM, the potential for lightweight FFF/FDM parts with less than 100% infill density, and the ability to recycle FFF/FDM printed parts after disposal [32]. Kellens et al. [42] compared the energy demands of polymeric SLS and metallic Electron Beam Melting (EBM). They found that SLS had a specific energy consumption (SEC) range of 107 to 145 MJ/kg, with waste powder contributing to nearly 50% of its environmental impacts. On the other hand, EBM's SEC values ranged from 60 to 375 MJ/kg, with the majority of energy consumed during the operational mode [42]. Similar other comparative results have been reported in the literature [16,36,41,43].

On the other hand, many articles have dedicated their focus to examining and contrasting the environmental impacts of diverse AM technologies in comparison to CM approaches. Priarone and Ingarao [9] conducted a comparative study on the environmental impacts of producing metal parts using CM and an integrated process combining AM with finish machining. Their findings indicated that the AM plus finish machining approach was more environmentally friendly, considering factors such as carbon dioxide gas emissions and energy consumption [9]. Huang et al. [11] evaluated the environmental advantages of shifting from CM to AM processes in the U.S. aircraft industry. Their findings revealed significant energy savings through AM fabrication compared to CM, with savings ranging from approximately 2 GJ for brackets to around 70 MJ for seat buckles. The reduction in energy consumption was primarily attributed to the lighter weight of AM parts, resulting in decreased airplane fuel consumption [11]. Similarly, other comparative studies have been reported in the literature [5,10,34,44–47]. Based on these studies, it can be concluded that whether AM exhibits higher or lower environmental impacts compared to CM approaches is primarily contingent on the specific criteria used for sustainability evaluation and the particular manufacturing method being substituted by AM. In addition to the insights provided here, readers interested in LCA studies in the context of AM are encouraged to explore the following review articles [48–50].

2.2. Influential Parameters and Strategies for AM Environmental Sustainability

A comprehensive analysis of the existing literature revealed that various AM parameters play a significant role in influencing its environmental performance. To identify these influential parameters, an extensive systematic review was conducted on articles obtained from two renowned academic databases, namely "Web of Science" and "Google Scholar". The gathered articles underwent a three-phase refinement procedure.

The first phase entailed implementing practical screening criteria to obtain insightful publications from the past years. To ensure high-quality publications, conference articles, commentaries, and working papers were excluded. The search phrase can be duplicated with the following searching sentence: "Topic: ("Sustainability" OR "Environment" AND "Additive Manufacturing" OR "3D Printing"); Time Span: 2001–2023; Language: "English"; Type: "Article" (searched on 21/03/2023)". This comprehensive search has yielded 650 articles, which were subsequently subjected to additional examination.

The subsequent phase involved a theoretical screening procedure to further narrow down the relevant articles based on specific criteria. This included studies exploring environmental sustainability in AM, encompassing the impacts of AM design and process parameters on material waste reduction, energy consumption, and environmental implications. Additionally, articles providing comprehensive overviews of AM's environmental sustainability trends and research gaps were considered. The screening process also included research addressing environmental sustainability within the AM context, even if not explicitly labeled as such, to identify potential future directions for integrating environmental sustainability into AM practices. At the end of this phase, the

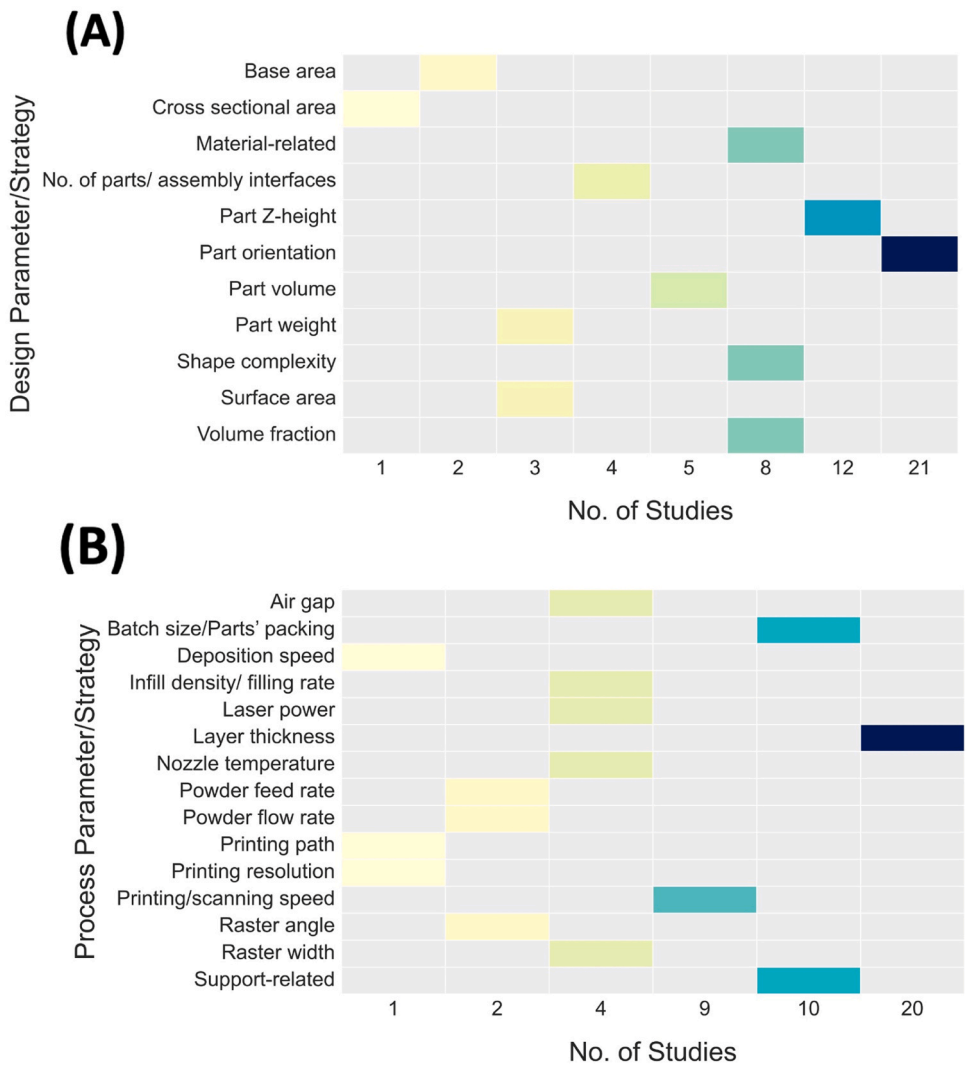

Fig. 2. Number of studies related to AM's environmental sustainability, categorized by A) design, and B) process parameters/strategies.

article count was reduced to 143.

In the final phase, the cited references from these 143 articles that met the selection criteria were used as a secondary source for a comprehensive literature analysis. This process unveiled 10 additional articles, bringing the total to 153 articles included in this systematic review of influential parameters. To facilitate article analysis, categories were established based on their relevance to the research focus, allowing for easy reference. Additionally, supplementary references were incorporated into the reference section to enhance the survey and offer further context.

Based on the findings of the systematic review conducted, research examining the impact of influential AM parameters and strategies can be classified into three primary categories. The first category comprises studies that analyze the impacts of design-related parameters and approaches. The second category involves research that investigates the influence of process-related parameters and support structures. Lastly, the third category encompasses studies that aim to understand the combined effects of AM design and process parameters through the concept of product-process co-design.

Within the first category, research has concentrated on investigating how geometry-related and material-related parameters/approaches affect the environmental sustainability of AM. Specifically, studies on the influence of part orientation [51,52], Z-height [53], surface area, cross-sectional area, and base area [54,55], weight [11], volume [36,56], topology optimization [33,57,58], cellular structures [54,59], shape complexity [36,55,60,61], and the number of parts (e.g., part consolidation [62–64] and parts segmentation [17]) on the environmental impacts of AM have been reported. With regard to the material-related parameters/strategies, studies have been conducted on examining the impact of material density [65,66], shrinkage rate [15], material emissions [15], biodegradability [67,68], and recyclability [68–70] on the environmental performance of the AM process.

Studies under the second category have explored the effect of process parameters and support structures on the environmental impacts of AM. A thorough examination of these studies revealed that fourteen process-related parameters (layer thickness [71,72], laser power [72–74], printing/scanning speed [72,74], deposition speed [75], powder feed rate [72–74], nozzle temperature [76–78], infill density [79,80], batch size/nesting efficiency [39,81], printing path [82], printing resolution [83], powder flow rate [74,75], raster width [84], raster angle [85], and air gap [86]) and five support related parameters/approaches (support height [16,56], support volume [82,87], filling strategy [17], optimized [82,88,89] and reusable [90] structures) were found to pose an impact on the environmental sustainability of AM.

The last category of studies has focused on analyzing the integrated impacts of AM design-and process-related parameters [18,19,91–93], or AM design, process-related parameters, and support structures [15,94] on the environmental sustainability of AM. Fig. 1 summarizes the various AM's environmental sustainability influential parameters/strategies. It should be noted that the influential parameters/strategies

depicted in Fig. 1 are applicable to all AM technologies. On the other hand, Fig. 2 (A) and (B) respectively provide an overview of the frequency that each of these influential AM design and process features/strategies was examined in the literature. Readers are encouraged to explore the following review article [95] for further insights on these influential features.

2.3. ML in sustainable manufacturing

In recent years, the field of sustainable manufacturing has witnessed a remarkable transformation with the integration of ML techniques. ML has shown tremendous potential in revolutionizing manufacturing processes and driving sustainability advancements. By leveraging large datasets, advanced algorithms, and predictive analytics, ML enables manufacturers to make data-driven decisions, optimize resource consumption, reduce waste, and enhance the overall environmental performance. Further, there has been a recent surge in the adoption of ML algorithms in the sustainable manufacturing field [96–98]. Through the use of ML, industries can automate sustainable knowledge acquisition processes which can be time-consuming to automate using other conventional approaches. To improve and maintain sustainability in the manufacturing domain, various types of knowledge-based systems (e.g., expert systems, fuzzy controllers, and intelligent scheduling) have been developed in the last few years [99]. ML has found applications in numerous sustainable manufacturing domains, including operational decision-making for machine systems [100], process parameters optimization for milling [101,102], energy/power consumption modeling for hard milling [103], production tools [104], and mask image projection SLA [105,106], sustainable planning and scheduling [107–109], energy prediction modeling for machine tools [110], and quality control for FDM [111] and metal AM [112]. Further, continuous maintenance in production lines can result in significant expenses. To overcome this, manufacturers have started to switch to ML-based condition monitoring and predictive maintenance for various conventional machining applications [113–116].

2.4. ML in LCA applications

Recently, there has been a growing inclination and focused endeavors toward leveraging ML for estimating LCA data. A number of studies in the literature have explored the feasibility of integrating LCA with ML to develop digitized alternative methods that support decision-making processes during the planning and design stages. These methods aim to provide assessments that can be conducted early in the design process, identify critical parameters influencing Life Cycle Impact Assessment (LCIA) metrics, and offer guidance for sustainability improvements. Li et al. [117] conducted a literature review to highlight recent advancements and challenges in addressing multidimensional links and spatiotemporal variations in LCA. They also introduced a new methodological framework, and practical recommendations for integrating big data with LCA, aimed toward enhancing the accuracy of indicator measurement and the efficiency of decision-making [117]. Ji et al. [118] were able to develop an effective method for accurately predicting the life spans of buildings by utilizing various ML prediction techniques. Four prediction models, namely Linear Regression (LR), Extreme Gradient Boosting (XGBoost), Light Gradient Boosting Machine (LightGBM), and Deep Neural Network (DNN) were employed to predict building life spans. Remarkably, even the basic LR model exhibited a robust prediction accuracy of 93.4%. Additionally, among the various ML models explored in this study, the DNN model demonstrated the highest prediction accuracy of 95.5%, surpassing the LR model by 2.2%. These findings collectively indicate that the utilization of ML models significantly improves the accuracy of building life span predictions compared to traditional approaches based on assumed values [118]. D'Amico et al. [20] employed Artificial Neural Network (ANN) to simultaneously assess the energy and environmental impacts of buildings' life cycles. Their database contained a collection of building models that have been simulated in different climatic conditions. It comprised 29 input parameters, including 13 energy-related data and 16 environmental data points. The database also provided seven output variables, consisting of one for heating energy demand and six commonly utilized indicators for evaluating the life cycle assessment of

Table 1
Summary of studies leveraging ML in LCA applications.

Field	Objective	ML Algorithm	Findings	Reference
Civil Engineering	-Predict the life spans of buildings.	- LR, XGBoost, LightGBM, and DNN.	-DNN demonstrated the highest accuracy (95.5%). -Compared to traditional approaches, ML models significantly improved the accuracy of building life span predictions based on assumed values.	Ji et al.[118]
	-Assess the energy and environmental impacts of buildings' life cycles.	-Various ANN's architectures.	-Optimal ANN architecture exhbited low RMSE, MAE below 5%, and R^2 close to 1.	D'Amico et al.[20]
	-Estimate land use changes in terms of greenhouse gas emissions following road construction.	- ANN and RF.	-RF was deemed a faster and a more effective approach in modeling the potential impacts of land use changes in terms of greenhouse gas emissions.	Larrea-Gallegos et al. [12]
Chemical Engineering	-Investigate the connections between LCIA values of chemicals and their molecular structures.	-DNN.	-The DNN model predicted a viable green chemical alternative, suggesting a promising approach for identifying eco-friendly alternatives in pharmaceutical processes.	Zhu et al.[22]
	-Estimate missing ecotoxicity hazardous concentrations 50% (HC50) for chemicals.	-Gradient Boosting Machine, ANN, SVM, RF, K Nearest Neighbors, and Adaptive Boosting.	-RF showed superior predictive performance.	Hou et al. [25]
	-Estimate LCA metrics for bio-based and biorefinery processes.	-ANN and DTs.	-Integrated use of ANN and DTs can support conventional LCA studies and enhance decision-making processes in early design stages.	Karka et al. [13]
Automotive Industry	-Predict greenhouse emissions of substituting glass fiber composites with natural fibers.	- LR, Decision Forest, Boosted Decision Tree, Bayesian Regression, Neural Network, and Poisson Regression.	-Neural network, Poisson model, and Decision Forests resulted in accurate predictions. -Despite the limited input data, ML deemed effective in predicting greenhouse emissions accurately.	Akhshik et al. [24]
Environmental Engineering	-Estimate missing unit process data.	-XGBoost, RF, ANN, and SVM.	-The model was able to classify zero and non-zero flows with a 0.79% misclassification rate even when 10% of the data was missing. For non-zero flows, R^2 was above 0.7 with less than 20% missing data.	Zhao et al. [23]

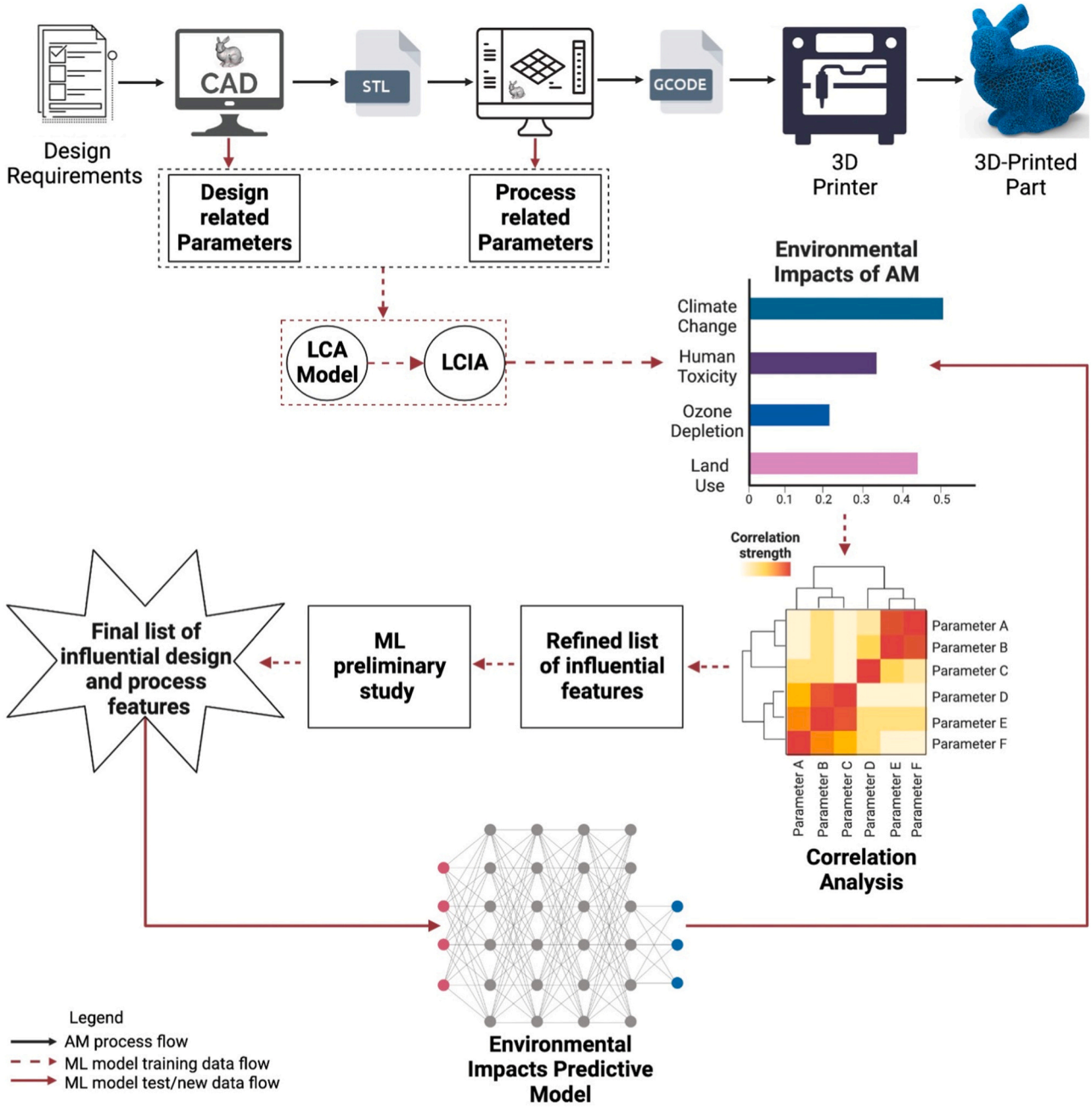

Fig. 3. The proposed framework for automating LCA for the AM process.

buildings. The accuracy of various ANN's architectures were examined. For each output, the optimal ANN demonstrated a low Root Mean Square Error (RMSE), Mean Absolute Error (MAE) below 5%, and a determination coefficient (R^2) close to 1 [20].

Zhu and co-authors [22] utilized ML to investigate the connections between the LCIA values of chemicals and their respective molecular structures. A total of 224 nonionic organic chemicals with known LCIA values were employed to build, train, and test predictive models using the DNN algorithm. Subsequently, the molecular descriptors of 30 similar chemicals were incorporated into the well-trained ML model to predict their LCIA values. The DNN model was able to predict a promising green chemical alternative. This approach promises to offer a guide to identify eco-friendly alternatives in pharmaceutical processes from large chemical databases, potentially reducing the need for experiments and associated costs [22]. Hou et al. [25] developed ML models to estimate missing ecotoxicity hazardous concentrations 50% (HC50) to calculate characterization factors for chemicals. Using the physical-chemical properties of chemicals and their mode of action classification, the authors were able to develop and compare six regression ML models: Gradient Boosting Machine, ANN, Support Vector Machine (SVM), Random Forest (RF), K Nearest Neighbors, and Adaptive Boosting. The findings indicated that the RF model exhibited superior predictive performance compared to other models [25].

Karka et al. [13] presented a data-driven framework that utilizes ML techniques to estimate LCA metrics for bio-based and biorefinery processes during the initial stages of the design process. The predictive model was developed using a limited amount of data. The study findings showed that the integrated utilization of ANN and Decision Trees (DTs) can provide support for conventional LCA studies and enhance the robustness of decision-making processes during the early stages of the process concept [13]. Akhshik et al. [24] have employed ML to predict the greenhouse emissions of substituting glass fiber composites with

light weighted natural fibers within the automotive industry. Six ML regression algorithms, namely LR, Decision Forest, Boosted Decision Tree, Bayesian Regression, Neural Network, and Poisson Regression were used to develop the predictive model. Results showed that Neural Network, Poisson model, and Decision Forests are all viable options for making accurate predictions. Further, despite the use of a limited amount of input data, ML was deemed suitable for predicting greenhouse emissions with acceptable accuracy [24]. In another investigation, Larrea-Gallegos et al. [12], estimated land use changes by developing an ML predictive model given a specific set of variables within a predetermined time frame. Two predictive algorithms were examined to model the potential impacts of land use changes in terms of greenhouse gas emissions following the construction of a road. Compared to ANN, RF proved to be a faster and a more straightforward approach in modeling the system being studied. While the availability of data remains a constraint, the study illustrates how ML models can complement decision-making based on LCA outcomes [12]. Zhao et al. [23] developed an ML model to estimate missing unit process data. They have employed a decision tree-based supervised learning approach, utilizing an existing unit process dataset (ecoinvent 3.1), to establish the correlation between the known information and the missing data. Various ML models including XGBoost, RF, ANN, and SVM have been adopted to generate the prediction model. The results indicated that the developed model can effectively classify zero and non-zero flows with a minimal misclassification rate (0.79%) even when 10% of the data is missing. For non-zero flows, the model was capable of accurately estimating their values with an R^2 above 0.7 when less than 20% of the data was missing in a unit process [23]. Table 1 provides a summary of these studies along with their findings. The exploration of these studies highlights the expansive utilization of ML, stretching its capabilities beyond conventional boundaries to address a wide array of environmental assessment challenges with remarkable efficacy.

3. The proposed DD-LCA framework

Despite the proven effectiveness of ML tools in various AM applications and in predicting LCA data of other research fields, the research community still lacks studies on the feasibility of ML algorithms to quantitively assess the environmental impacts of the AM process. Several obstacles contribute to this gap, one of which is the absence of a standardized and automated LCA framework designed for AM. Another obstacle to automating LCA for AM is the limited availability of publicly accessible datasets. In certain domains, like optical character recognition with MNIST [119] or image recognition with ImageNet [120], substantial datasets exist for training ML models, leading to significant advancements in these areas. On the other hand, this is not the case for AM. While there are a few platforms, such as additive manufacturing materials databases, IEEEDataPort, DOE Data Explorer, and DATA.GOV, that provide some datasets related to AM, they remain quite restricted in scope, primarily focusing on particular AM technologies and design/-process parameters [121,122]. The expensive process of collecting training data in AM is another challenge that hinders automating LCA for AM. To date, there is no harmonized practice for extracting design and process features in AM. Some design (i.e., volume, surface area, weight, etc.) and process (layer thickness, infill density, printing speed, support volume, etc.) data can be manually extracted using slicing software, however, this can be expensive and time-consuming [122]. While certain studies [56,106] in the literature have employed various feature extraction algorithms for this purpose, a standardized approach has not yet been established. The lack of sufficient expertise in identifying influential features is another challenge that impedes the adoption of ML-assisted LCA for AM. Certain AM design and process variables can greatly impact the environmental performance of AM, while others may have a less pronounced effect [122]. To address some of these challenges, the authors deemed it necessary to develop a methodological framework to unlock the potential of ML tools in accurately predicting the environmental impact of AM processes. The ultimate goal of this framework is to facilitate the transition toward automated LCA for AM technologies.

Fig. 3 illustrates the proposed framework for supporting automated LCA for AM. The framework comprises two primary workflows: the general AM process and the environmental impact prediction process. The general AM process begins with the design requirements, which are then mapped to specific design features in a Computer-Aided Design (CAD) file. To enable printing, the CAD file is converted into a STereo-Lithography (STL) file containing the geometric information. Next, process parameters are selected and the STL file is sliced. The 3D printer then executes the printing job based on the extracted G-Code. The environmental impact prediction process involves selecting a preliminary set of influential design and process-related parameters/features (Fig. 1) that pose an impact on the environmental performance of AM. These features can then be instantiated using parts with various geometries and materials. The features' values can then be obtained either manually using slicing software or programmatically through data extraction algorithms. The next step involves conducting LCA to generate a comprehensive set of sustainability impact indicators. The subsequent stage involves using correlation analysis to spot correlations between features. Based on the correlation analysis results, a refined list of influential features is to be derived. The following step involves an ML-based preliminary study for a more refined feature selection evaluation. Based on the outcomes of this preliminary study, a final list of influential features is anticipated. The next stage entails normalization, training, and building the environmental impact predictive model. The performance of various ML models is then compared and evaluated. Given that the environmental impact categories are continuous variables, it might be reasonable to start with a simple regression prediction model, which can serve as a suitable baseline model. Supervised learning regression models can then be compared against the baseline model to assess their prediction performance.

4. DD-LCA model construction

This section presents the implementation of the proposed DD-LCA framework, utilizing the FFF AM process as a case study. It also includes the construction of the DD-LCA dataset for training, data preprocessing, comparative evaluation of various ML algorithms, and feature selection evaluation. It should be advised that with appropriate modifications, the proposed methodology exhibits the potential to be generally applied to other AM processes.

4.1. Data collection and construction of DD-LCA training dataset

To initiate our exploration, it is essential to extract an initial list of influential features for the FFF AM process from the comprehensive compilation presented in Fig. 1. As evident from Fig. 2 (A) and (B), certain influential features (e.g., part orientation and layer thickness) have gained considerable research attention. Conversely, other features (e.g., base area, cross-sectional area, and air gap) have received relatively less exploration. This could be attributed to their minimal environmental impact or the need for more extensive research to fully comprehend their influence on AM's environmental performance. Until further investigations are conducted to understand the environmental repercussions of such features, it may be prudent to overlook or disregard them. Thus, to select a preliminary set of influential design and process-related features for the FFF technology, practitioners could start with a set of five design features including part volume, weight, Z-height, surface area, and filament density, along with seven process features consisting of layer thickness, printing speed, nozzle/printing and platform temperatures, infill density, support height, and support volume.

The primary data for this study is then obtained by instantiating these 12 selected features using parts with different levels of shape

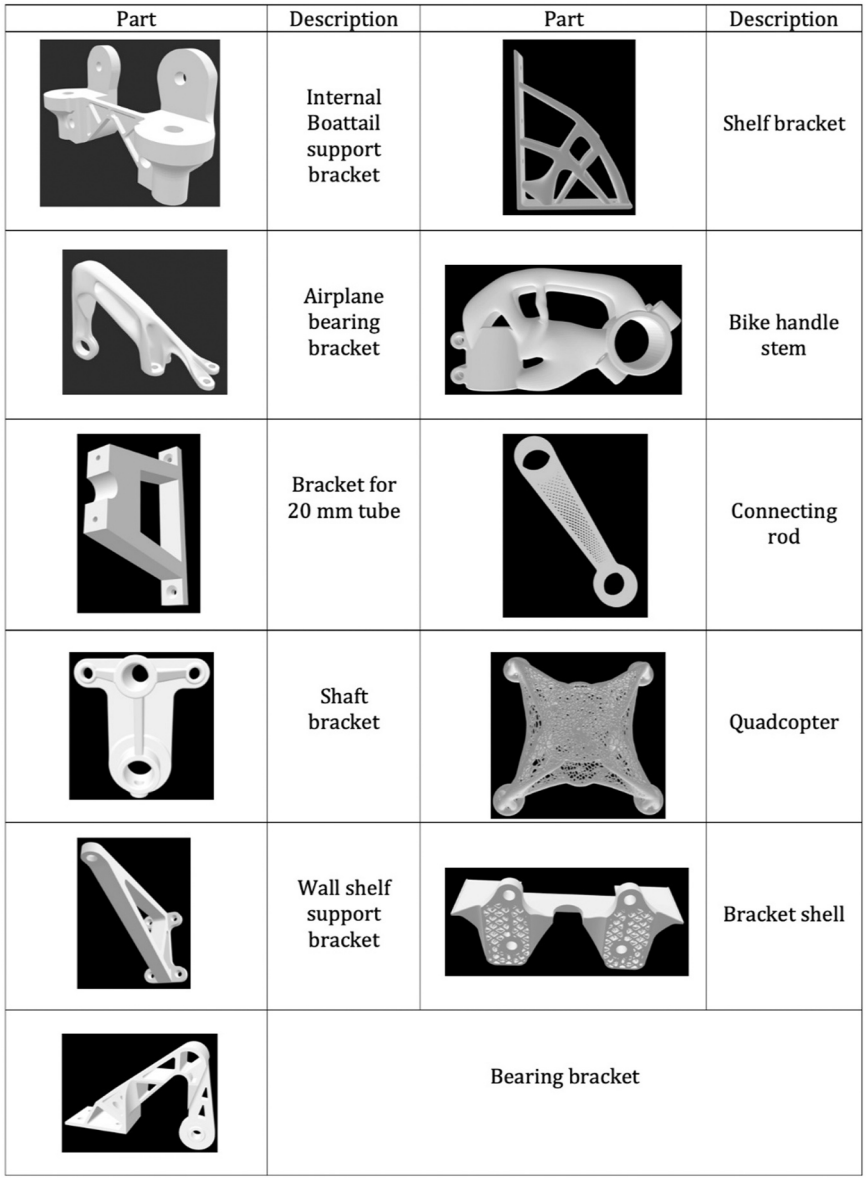

Fig. 4. An overview of the parts inventory.

Table 2
Statistical summary of the initially selected influential features.

AM Design Features					
Feature	**Unit**	**Range**	**Mean**	**Standard Deviation**	**Source**
Part volume	cm^3	11.83-178.1	49.01	36.54	3D CAD software SolidWorks®.
Part weight	N	0.12-1.8	0.54	0.40	Open-source software Ultimaker Cura.
Part Z-height	mm	20-179.2	65.45	40.48	Open-source software Ultimaker Cura.
Part surface area	cm^2	155.8-650.6	360.80	171.49	3D CAD software SolidWorks®.
Filament density	g/cm^3	1.04,1.24	1.13	0.10	Vendor data.
AM Process Features					
Feature	**Unit**	**Range**	**Mean**	**Standard Deviation**	**Source**
Layer thickness	mm	0.1-0.6	0.146	0.12	-
Printing speed	mm/s	40-55	48.87	3.92	[124,125].
Nozzle temperature	°C	210,240	225.15	15.04	[126].
Platform temperature	°C	60,105	82.72	22.55	[126].
Infill density	%	20-100	39.31	29.48	-
Support height	mm	9.03-154.1	39.05	31.61	Open-source software Ultimaker Cura.
Support volume	cm^3	0.288-115.81	16.41	19.9	Open-source software Ultimaker Cura.

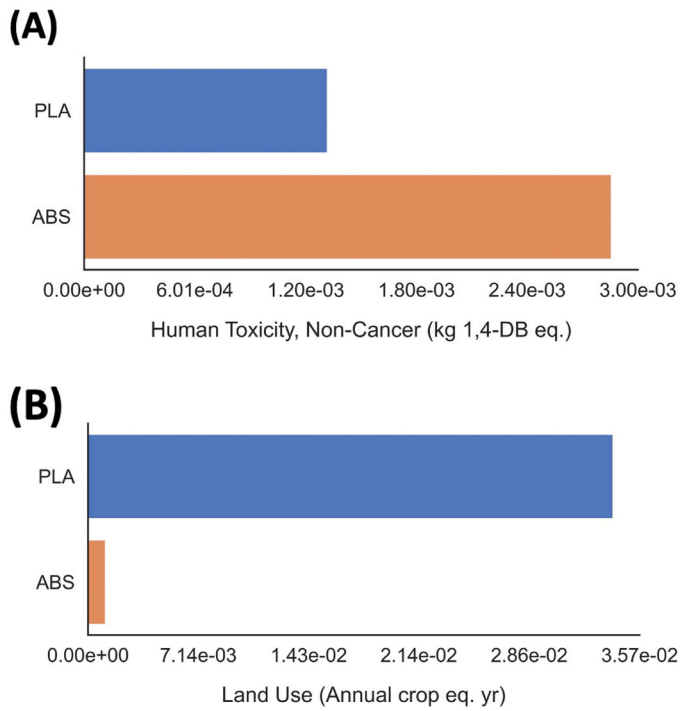

Fig. 5. A comparison between LCA of PLA and ABS for A) the human toxicity, non-cancer, and B) the land use impact categories.

complexity [123]. Having said that, Fig. 4 presents the parts inventory, depicting an inclusive list of the parts utilized in this study. With that in mind, some of these parts have been topology optimized (e.g., shelf bracket) while others have been optimized using cellular structures (e.g., connecting rod and quadcopter). Using the open-source software Ultimaker Cura, estimations for the material consumption and printing time for each combination of AM design and process features were obtained. Further, the energy consumption was estimated by adopting the approach proposed by Li et al. [32]. For each part, two different printing orientations were considered, and two various filament materials were investigated: Acrylonitrile Butadiene Styrene (ABS) and Poly(lactic acid) (PLA). Table 2 presents a comprehensive statistical summary of the 12 selected features, including the respective sources from which their values were obtained.

The next phase involved conducting an LCA study according to the guidelines provided in the ISO 14040 standard [127]. The system boundary governs which unit processes are included or excluded in the LCA. Due to the data-intensive nature of the Cradle-to-Cradle system boundary and the high degree of assumptions and uncertainties that are usually associated with such a scope, the system boundary adopted in this study is Gate-to-Grave. In this investigation, the system boundary begins with the arrival of raw materials at the manufacturing facility's entrance gate, extends through the manufacturing process, the product's use phase, and ultimately concludes with recycling of the wastes. This holistic view enables a thorough analysis of environmental impacts across all these stages and avoids potential biases that may arise from focusing on specific stages or ignoring certain impacts [128,129]. The analysis of the LCA study was undertaken using the GaBi ts LCA software. The modeled system covered the following steps: plastic production, extrusion of the 3D filament, additive manufacturing process, and recycling of the wastes. PLA/ABS Plastic production process was modeled using the integrated production process in the LCA software. The extrusion process was modeled using total material consumption as the input and the outputs consisted of the same amount of material as extruded filament. The 3D printing process was modeled taking into account the energy consumption and the extruded filament as inputs

Table 3
A sample data point in the constructed training dataset.

Features		
Design Parameter	**Unit**	**Amount**
Part volume	cm^3	11.93
Part weight	N	0.145
Part Z-height	mm	20.56
Part surface area	cm^2	432.8
Filament density	g/cm^3	1.24 (PLA)
Process Parameter	**Unit**	**Amount**
Layer thickness	mm	0.1
Printing speed	mm/s	50
Nozzle temperature	°C	210
Platform temperature	°C	60
Infill density	%	20
Support height	mm	16.373
Support volume	cm^3	15.081
Target Variables		
LCA Impact Category	**Unit**	**Amount**
Climate change	kg CO_2-eq to air	0.110
Fine particulate matter formation	kg PM2.5-eq to air	0.0000473
Fossil resource scarcity	kg oil-eq	0.0214
Water use	m^3 water-eq consumed	0.173
Freshwater ecotoxicity	kg 1,4-DCB-eq to freshwater	0.000202
Freshwater eutrophication	kg P-eq to freshwater	0.000000341
Human toxicity: cancer	kg 1,4-DCB-eq to urban air	0.00165
Human toxicity: non-cancer	kg 1,4-DCB-eq to urban air	0.00171
Ionizing radiation	kBq Co-60-eq to air	0.000638
Land use	$m^2 \times$ year annual cropland-eq	0.0396
Marine ecotoxicity	kg 1,4-DCB-eq to marine water	0.000119
Marine eutrophication	KgN-eq to marine water	0.0000032
Mineral resource scarcity	kg Cu-eq	0.000696
Photochemical oxidant formation: terrestrial ecosystems	kg NOx-eq to air	0.000184
Photochemical oxidant formation: human health	kg NOx-eq to air	0.000183
Ozone depletion	kg CFC-11-eq to air	0.000000102
Terrestrial acidification	kg SO_2-eq to air	0.000144
Terrestrial ecotoxicity	kg 1,4-DCB-eq to industrial soil	0.0140

while the additively manufactured part in addition to the support structure were considered as the outputs. Finally, 34% of the total material consumption was assumed to be mechanically recycled [130]. All inputs (total material consumption and energy consumption) and outputs (additively manufactured part and support structure) were included within the system boundary. One count of an additively manufactured part with a known volume was defined as the functional unit. On the other hand, selecting the appropriate impact assessment methods in LCA holds significant importance. ReCiPe offers a harmonized implementation of cause-effect pathways for the calculation of both midpoint and endpoint characterization factors [131]. Although the aggregation of results into a single score in the endpoint approach facilitates easier interpretation by decision-makers as well as better communication to the public, they are associated with a higher degree of statistical uncertainty, in comparison to the midpoint. This can be attributed to the assumptions and data gaps stacking up along the cause-effect chain. Thus, the environmental assessment was conducted according to the characterization factors reported in the ReCiPe (World-H) 2016 midpoint method. A hierarchical (H) perspective is implemented, providing a consensus model based on common policy principles regarding time frame and other issues [132].

Findings of the LCA were as expected, that is the most sustainable AM design and process features (e.g., lowest volume, lightest weight, shortest Z-height, highest layer thickness etc.) resulted in the lowest

environmental impacts. For the same combination of AM design and process parameters (excluding material-dependent parameters), a comparison has been done to understand the effect of filament material choice on the environmental impact categories. Fig. 5 (A) shows a comparison of the human toxicity, non-cancer impact category between PLA and ABS. Results showed that utilizing PLA as a filament material can result in a relatively lower non-cancer human toxicity impact compared to ABS. The same trend has been also observed for the terrestrial ecotoxicity impact category. On the other hand, ABS emerged as a better option due to its relatively comparable or superior performance across all other impact categories. For instance, ABS resulted in a lower land use impacts in comparison to PLA (Fig. 5 (B)). This might be attributed to the fact that the production of PLA requires the cultivation of crops, such as sugarcane or corn. The cultivation of these crops can result in significant land use, which might intensify freshwater eutrophication due to nutrient runoff from fertilizers, leading to oxygen-depleting algal blooms. Additionally, the pesticides and herbicides used in PLA crop cultivation can elevate freshwater ecotoxicity, posing threats to aquatic life [133–135]. This might also explain the higher freshwater eutrophication and ecotoxicity impacts of PLA in comparison to ABS. In contrast, ABS production, being petroleum-derived, does not have the same direct routine impact on the land use and freshwater categories, though it carries its own environmental concerns. Although PLA possesses biomaterial characteristics, its sustainability benefits can be more pronounced if a more detailed Cradle-to-Grave LCA approach is utilized, with emphases on the role of biodegradability in reducing the environmental footprint.

At the end of this stage, a diverse training dataset consisting of 200 data points corresponding to 11 different parts was constructed. Each data point comprises a unique combination of AM design and process parameters (features) along with its corresponding 18 impact categories (target variables). Table 3 shows an example of a single data point that corresponds to the quadcopter part printed using PLA.

4.2. Data Pre-processing

Data processing is an integral required step for cleaning the data and making it suitable for an ML model to increase the efficiency and accuracy. Therefore, all entries with 0 values, Not a Number (NaN), and string variables have been removed. As shown in Table 2, the entries in the dataset used in this study exhibit very different orders of magnitude because of the choice of different units. It has been accepted as a common practice that when the features have varying scales, the effect of the bigger number will dominate the outcomes; hence, a normalization/feature scaling step is usually essential to transform the data into a feasible range [24]. The data was preprocessed by employing Scikit-Learn's pre-processing and scaler functions. Using the MinMaxScaler method provided with the pre-processing package, the training and testing datasets were normalized to values between 0 and 1. Furthermore, a robust hyperparameter tuning using RandomizedSearchCV function followed by GridsearchCV was done to seek optimal model parameters. After tuning the parameters, only the optimum combinations were used for further analysis. Each data point was then randomly divided into two groups of 80% and 20% destined for training and testing respectively. All proposed models were trained and tested using the same random-generation seed.

4.3. ML algorithms

In ML, the conditions needed to attain optimal outcomes is contingent upon the characteristics of the collected data as well as the nature of the problem. Hence, it is essential to apply ML techniques that are specific and suitable to the problem. Since the 18 impact categories are continuous variables, a simple regression prediction model was constructed first and considered as a baseline model against which the performance of other ML models was compared. Other regression algorithms including multivariate polynomial, DTs, RF, support vector regressor, XGBoost, and multi-layer perceptron were also adopted to construct the prediction model.

4.3.1. Linear regression (LR)

For the baseline model, the Scikit-Learn Python library was utilized to implement an LR model. An LR model seeks to capture and describe the relationship between the features (x) and target variables (y) through fitting a linear equation ($\widehat{y} = w_1x_1 + w_2x_2 + \ldots + w_nx_n + b$) to the data. Scikit-Learn's LR module builds a model by calculating the pseudo-inverse matrix via singular value decomposition [118].

4.3.2. Multivariate polynomial regression (MPR)

Polynomial regression that is applied to a single regressor variable is called simple polynomial regression. On the other hand, when the polynomial regression is computed on multiple regressor variables this is referred to as MPR. MPR offers an efficient way to describe complex input-output relationships. Such complex relationships are usually non-linear and highly dimensional. A second-order MPR for two features can be expressed as ($\widehat{y} = w_1x_1 + w_2x_2 + w_{11}x_1^2 + w_{22}x_2^2 + w_{12}x_1x_2 + b$) where w_1, w_2 are the linear effect parameters, w_{11}, w_{22} are the quadratic effect parameters and w_{12} is the interaction effect parameter [136,137]. Iterations for MPR with degrees 2–10 were constructed to seek the optimum MPR degree that reflects the best performance. Scikit-Learn's PolynomialFeatures was used to generate polynomial and interaction features.

4.3.3. Decision trees regressor (DTR)

DTs are one of the most widely employed practical approaches for supervised ML. DTs can be employed to solve both classification and regression problems. A DT is a hierarchical model that comprises decision rules, which recursively split independent variables into homogeneous regions or zones. The goal of a DT model is to generate a collection of decision rules that can be employed to forecast the target variable based on the independent features. In DT modeling, an empirical tree signifies a segmentation of the data achieved through the application of a series of basic rules. A DT can be visualized as a piecewise constant approximation. Through the repetitive process of splitting, the generated set of rules can then be used for prediction. A DT consists of three types of nodes. The root node serves as the initial node, representing the entire sample, and it can be further divided to generate additional nodes. The interior nodes on the other hand are those nodes that represent the features of the dataset. The branches represent the decision rules. Finally, the leaf nodes represent the final outcomes or predictions. DTs are a non-parametric model that is easy to understand and interpret without distributional assumptions. Furthermore, DTs simplify the complex relationship between the features and target variables by dividing the original features into significant subgroups [138,139]. DTs are characterized by ease of interpretation, stability, and high accuracy. Yet, DTs are prone to overfitting, specifically when the tree is particularly deep, and the dataset is small. DTR was generated using Scikit-Learn's DecisionTreeRegressor.

4.3.4. Random forest regressor (RFR)

RF is an extended variant of bagging, which fits various trees using bootstrap resampled versions of the training data. The prediction is then obtained by taking the average of each tree's results. RF is an ensemble learning method that enhances bagging by randomly selecting subsets of features during the training of each individual DT within the RF. The correlation between DTs is also reduced by randomly selecting candidate variables. Moreover, RF has a strong capability to mitigate overfitting because the final result is derived from averaging the predictions of multiple low-correlated DTs [23]. Scikit-Learn's RandomForestRegressor was used to generate the RFR model.

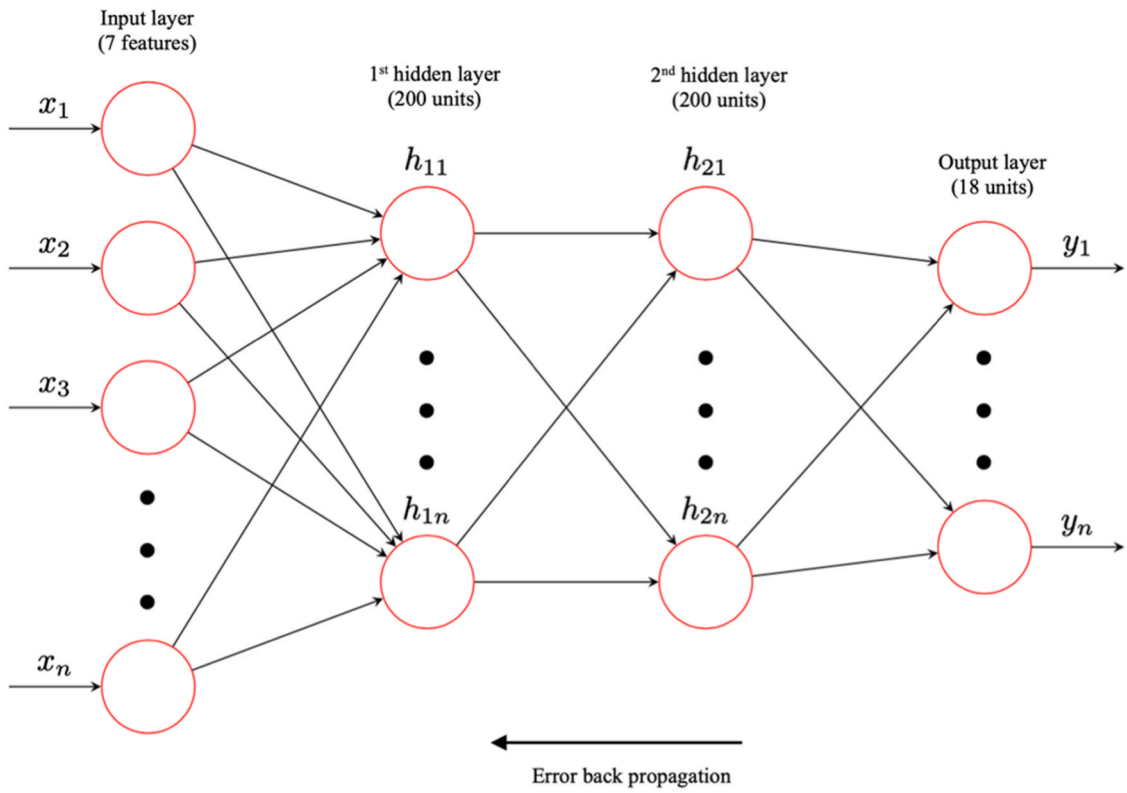

Fig. 6. Visual representation of the structure of the constructed MLP.

4.3.5. Support vector regressor (SVR)

SVR is an extension of the widely known SVM model that is utilized in multivariate regression problems. SVR is a prevailing algorithm that offers the flexibility of the error tolerance through an acceptable error margin and a satisfactory adjustment that exceeds the acceptable error rate. In this model, a nonlinear kernel function is employed to transform the data into a feature space of higher dimensionality. It then seeks a decision boundary (i.e., hyperplane), that minimizes errors within this transformed space. Dissimilar to other regression algorithms which try to minimize the error between the actual and predicted values, SVR attempts to fit the best line within a threshold value. This threshold value corresponds to the distance separating the hyperplane and the boundary line [23,140]. To develop the SVR model, Scikit-Learn's MultiOutputRegressor was used followed by sklearn.svm.SVR.

4.3.6. Extreme gradient boosting (XGBoost)

XGBoost is a boosting-based algorithm that follows the principle of combining weak classifiers to form a stronger classifier. The basic idea behind XGBoost is to iteratively train a series of weak learners, typically DTs, and then strategically combine their predictions to improve the overall performance. Each weak learner focuses on the samples that were misclassified or have high residuals from the previous iterations, allowing the model to learn from its mistakes and make better predictions. By using a combination of weak learners, XGBoost effectively handles complex relationships between features and targets, capturing both linear and non-linear patterns in the data. It also incorporates regularization techniques to prevent overfitting and optimize the model's generalization capabilities. The algorithm employs gradient boosting, which involves iteratively fitting new models to the residuals of the previous models, gradually reducing the errors and improving the overall accuracy. XGBoost further enhances this process by introducing additional enhancements such as parallelization, handling missing values, and tree pruning. With its robustness, scalability, and ability to handle large datasets, XGBoost has gained popularity in the ML community and has been widely used in various domains [141]. In this research, dmlc/XGBoost's XGBRegressor was used to create the XGBoost model.

4.3.7. Multi-layer perceptron (MLP)

MLP is a supervised ML algorithm that learns a function $f(\cdot) : R^m \rightarrow R^o$ by training on a dataset where m and o are the numbers of dimensions for the input and output respectively. MLP is a feedforward DNN which composes of multiple layers (i.e., input layer, hidden layers, and output layer) of "neurons". MLP can learn a non-linear function approximator for either regression or classification given a set of features and target variables. Unlike logistic regression, MLP can have one or more non-linear layers (hidden layers) between the input and output layers [23, 142]. In this study, Scikit-Learn's MLPRegressor was used to predict the eighteen environmental impact categories. Two hidden layers were constructed and used to minimize the square error between the predicted and actual values. MLP was trained using backpropagation and the rectified linear unit (ReLU) was employed as the hidden layer's activation function. Adam optimizer - a stochastic gradient-based optimizer was also used as the gradient boost optimizer [142]. Fig. 6 depicts a visual representation of the adopted MLP.

4.4. Feature selection evaluation

Feature selection is of paramount importance in ML due to its various advantages. One of its key benefits is the improvement of model performance. By selecting the most relevant features, noise and irrelevant information can be eliminated, enabling the model to focus on the most informative attributes. Consequently, this can lead to enhanced accuracy, better model generalization, and improved overall performance. Additionally, feature selection helps mitigate overfitting by reducing the complexity of the model and preventing it from learning spurious correlations. Moreover, selecting a subset of meaningful features reduces computational requirements, resulting in faster training and inference

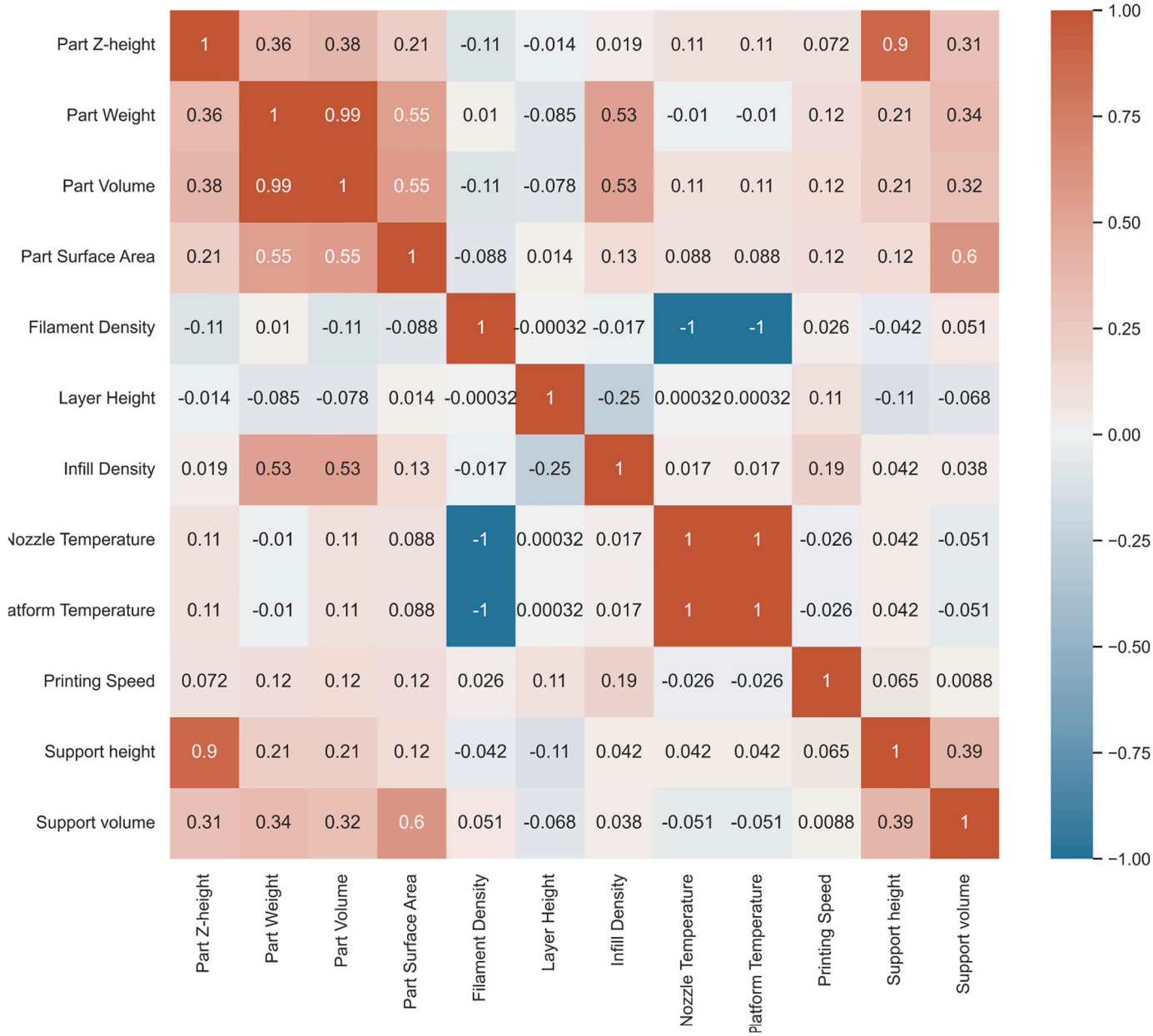

Fig. 7. Correlation analysis heat map.

Table 4
Summary of features reflecting very high, high, and moderate correlation.

Correlation coefficient	Feature 1	Feature 2
Very high (0.9-1.0)	Part weight	Part volume
	Filament density	Platform temperature
	Material density	Nozzle temperature
	Nozzle temperature	Platform temperature
	Part Z-height	Support height
High (0.7-0.9)	Support volume	Part surface area
Moderate (0.5-0.7)	Part weight	Infill density
	Part volume	Infill density
	Part weight	Part surface area
	Part volume	Part surface area

times. While it is important to strike a balance between selecting informative attributes and retaining valuable information, different feature selection techniques can be employed to suit the specific requirements of the problem and dataset characteristics [143,144]. The forthcoming sections comprehensively explore feature selection evaluation, focusing on specific aspects such as correlation analysis and the development of refined and final lists of influential features.

4.4.1. *Correlation analysis and feature refinement*

Correlation analysis serves as a valuable tool to explore and unravel the interrelationships among key variables pertaining to AM's environmental sustainability. This study utilizes the Pearson correlation coefficient to assess the correlation between features. Pearson correlation coefficient is determined by dividing the covariance of two variables by the product of their standard deviation [145,146]. The effectiveness of the Pearson coefficient in detecting correlations between features has been demonstrated in multiple studies [145,147,148]. Fig. 7 depicts a heat map for the correlation analysis result. Table 4 represents a summary of those features that exhibit very high, high, and moderate correlations. Upon a closer examination of the findings, it becomes evident that both the printing and platform temperatures exhibit a perfect positive correlation (+1.0). Additionally, the filament

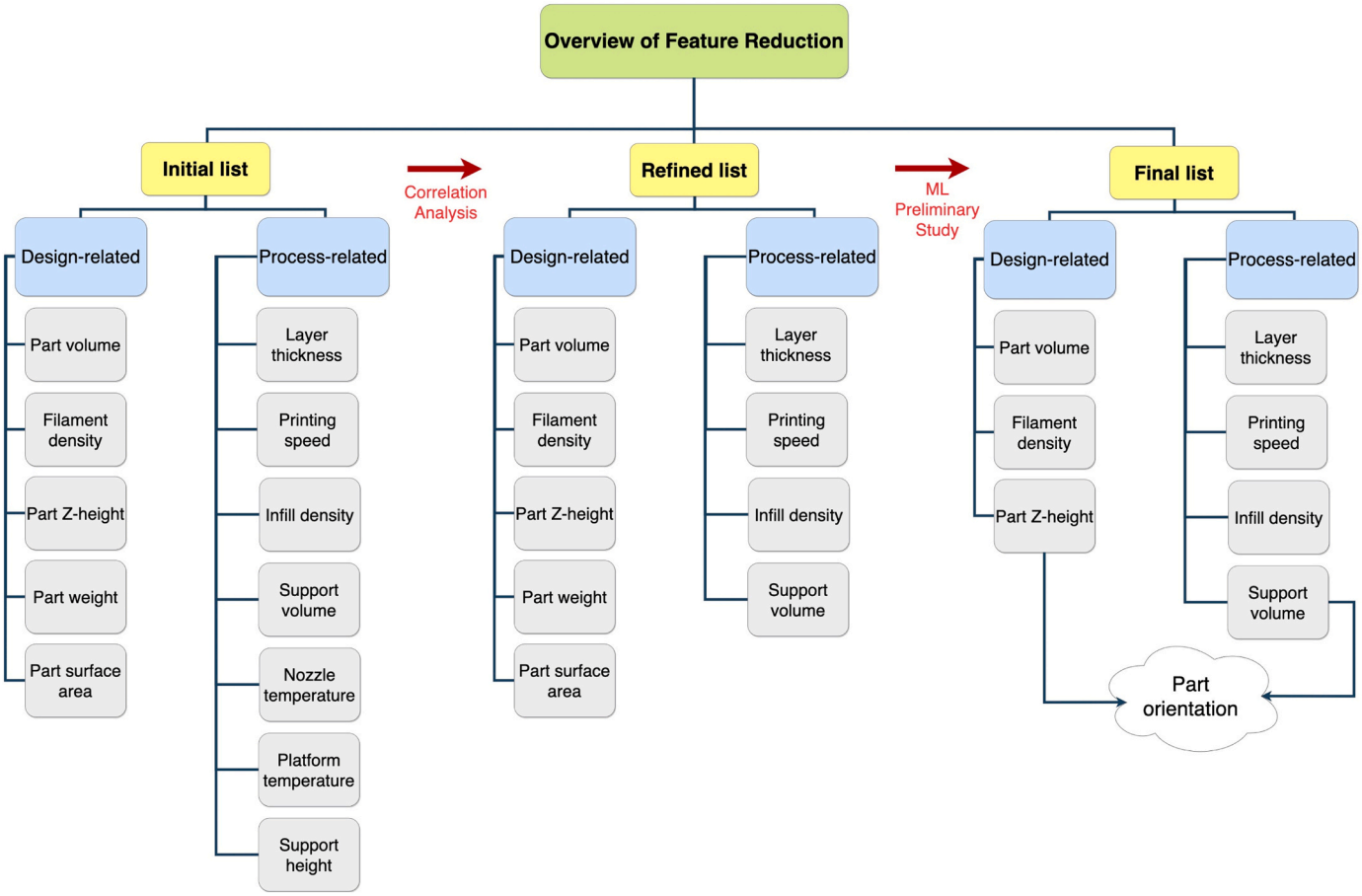

Fig. 8. Summary of feature reduction analysis.

density displays a perfect negative correlation (−1.0) with the nozzle and platform temperatures. Different filament materials have unique thermal properties, such as specific heat capacity, glass transition temperature, and melting point. A filament's density can often be an indicator of its composition, and thus, its thermal properties. To ensure good-quality prints, the printing and platform temperatures need to be adjusted based on these properties [149–151]. For instance, filaments with higher densities might exhibit a higher melting point and thus need more heat to maintain a molten state that allows for smooth extrusion and proper layer bonding. Further, filaments with various densities adhere differently to the print platform. For example, materials with higher densities often require a higher platform temperature to prevent warping and ensure good adhesion [150]. In addition, the degree of melting fluidity and shrinkage can be influenced by the filament density. To counteract these effects, the printing and platform temperatures are often adjusted based on the filament density [150,152]. Thus, given that these two temperature-related features are dependent on the filament density, it may be reasonable to consider excluding the nozzle and printing temperatures from the list of refined influential features. The findings also indicate a very high correlation (0.9–1.0) between the part Z-height and the support height. Consequently, it may be more appropriate to drop the support height from the narrowed-down list of features, as the height of the support is determined by the Z-height of the part. Further, it was found that the support volume and part surface area showed a moderate correlation (0.5 to 0.7). Similarly, the infill density demonstrated a moderate correlation with both the part weight and volume. Likewise, the part weight, volume, and surface area exhibited moderate correlations with each other. Thus, our refined list of influential features consisted of nine features, encompassing five design parameters (part volume, weight, Z-height, surface area, and filament density) and four process parameters (layer thickness, printing speed, infill density, and support volume). It is worth mentioning that the limitation of this type of analysis is that it cannot determine the causality between two independent variables. For instance, in the case of part weight and volume, which are very highly correlated, this analysis does not give enough insights into which one of these two features is a redundant parameter. Nonetheless, correlation analysis was employed in this study because, to the best of the authors' knowledge, this is the first study to employ ML toward automating LCA for AM. Thus, the authors aimed to present interpretable results to the research community by avoiding any feature transformation and data variability loss that are usually involved in other dimensionality reduction methodologies (i.e., principal component analysis).

4.4.2. *Final list of influential features*

Due to the limitations of correlation analysis and for a more refined feature selection evaluation, a preliminary study using various ML models corresponding to different combinations of the very high, high, and moderately correlated features was deemed necessary. Thus, the ML algorithms discussed earlier were employed to develop predictive models using various iterations. To illustrate the process, the first iteration focused on developing a predictive model for the 18 environmental impact categories using all the nine features in our refined list of influential features. In the second and third iterations, eight features were considered (i.e., one of the part weight and part volume, which are very highly correlated, was removed in each iteration). Based on the evaluation of the various feature selections, it was decided to continue with 7 features only: three of which are AM design parameters (part volume, Z-height, and filament density) while the remaining four are AM process parameters (layer thickness, printing speed, infill density,

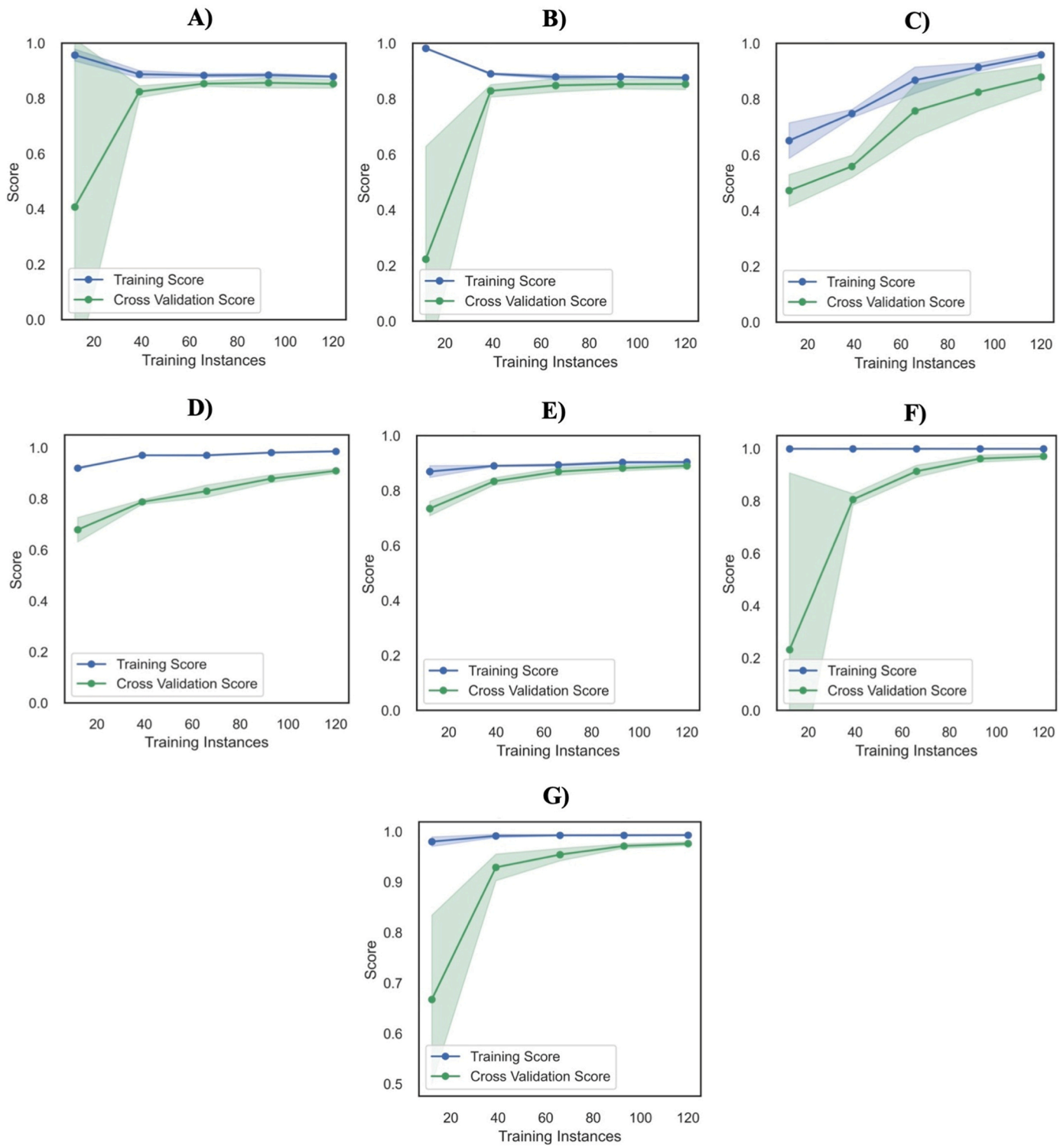

Fig. 9. Learning curves for A) LR, B) second-degree MPR, C) DTR, D) RFR, E) SVR, F) XGBoost, and G) MLP. Note: The solid lines represent the mean scores, while the shaded regions indicate the variability of scores (one standard deviation from the mean). The score used is R^2.

and support volume). It is noted that the Z-height of the part and the support volume were chosen as indicators of the part orientation influence. Fig. 8 depicts an overview of the feature reduction analysis.

5. Performance evaluation of the DD-LCA model

This section presents the performance evaluation of the DD-LCA model. In this section, we discuss the evaluation metrics employed to assess the model's performance and provide analysis and discussion of the obtained results. The aim is to gain a thorough understanding of the model's effectiveness and conduct a comparative analysis of the performances of the seven different ML algorithms to determine the most suitable algorithm to address the problem at hand. The section concludes by evaluating the model's generalizability on unseen data and identifying the environmental hotspots.

Table 5
Summary of the underfitting/overfitting analysis.

Model	Average R^2 for the training data	Average R^2 for the testing data	Average RMSE for the training data	Average RMSE for the testing data
LR	0.87	0.82	0.070	0.080
MPR (degree 2)	0.98	0.97	0.025	0.031
DTR	0.96	0.86	0.040	0.070
RFR	0.98	0.92	0.020	0.060
SVR	0.89	0.85	0.065	0.068
XGBoost	0.99	0.98	0.0020	0.026
MLP	0.99	0.97	0.020	0.030

5.1. Evaluation metrics

The phenomena of overfitting and underfitting play a vital role in the performance and reliability of ML models. Examining these phenomena provides insights into the model's ability to generalize beyond the training data. In this study, every model was assessed for underfitting/overfitting using k-fold cross-validation (CV). The entries in the dataset were split into five folds after they have been randomly shuffled. For each fold, one group of data was taken as a holdout or a test dataset while the remaining groups were treated as training dataset. Each model was then fitted on the training set and evaluated on the testing entries. This was followed by model's assessment and evaluation. The process was repeated for all the other folds. Prediction outcomes are often assessed using evaluation metrics such as the mean square error (MSE) and its square root variant, RMSE, or alternatively, the MAE and its percentage variant, the mean absolute percentage error (MAPE) [153]. In this work, RMSE and R^2 are employed to assess the ML models against underfitting/overfitting. RMSE is the square root of the quadratic mean of the difference between predicted and expected values. RMSE is chosen due to its robust performance to the effect of outliers and their errors. Although the dataset is normalized and preprocessed, there is still a chance for a few large entries to distort the model's estimation as a result of their large volume and variance. Hence, it is essential to utilize a robust metric like RMSE that accounts for generalized predictions. Besides prediction precision, it is also necessary to assess the extent to which the regression models accurately represent the observed values and the distribution of environmental impacts. There are arguments in preceding studies that symmetric mean absolute percentage error (SMAPE) should be employed for such criteria; nonetheless, more recent studies claimed the superiority of R^2 over SMAPE [118,153]. R^2 evaluates the model's accuracy in comparison to the actual data points. Thus, the average training and testing values of R^2 and RMSE for the five folds were considered to examine the models against underfitting/overfitting.

5.2. Result analysis and discussions

Learning curves provide valuable insights into how well a model generalizes and whether it exhibits signs of overfitting or underfitting. They also provide indications of how a model learns and improves over time as more data is fed into the training process. Fig. 9 depicts the learning curve analysis for all the models employed in this investigation. Overall, all models exhibit a small gap between the training and validation curves, suggesting that the models generalize well to unseen data. Further, the close alignment between the training and validation curves across all models indicates that that they are not prone to overfitting or underfitting. Moreover, all models were able to successfully learn and capture the underlying patterns and relationships in the data. This was evidenced by the gradual improvement in the validation curve as the number of training instances increased.

Table 5 shows a summary of the underfitting/overfitting analysis, displaying the average values of R^2 and RMSE for both training and testing across the five folds. The results suggest that LR, second-degree MPR, SVR, XGBoost, and MLP exhibited the least amount of overfitting, as their validation performance closely matched their training performance. All these five models converged quickly and achieved stable performances with minimal fluctuations. Further, the tight alignment between the training and validation curves in these models suggests that they are effectively generalizing from the available data. This close convergence indicates that the models have reached a point where the addition of more data is unlikely to result in significant improvements to their performance. In contrast, the DTR and RFR models exhibited a lack of convergence in their learning curves, indicating an unstable performance and suggesting the potential for improvement with additional data.

Table 6
Overview of the performance of different models.

Model	Average R^2	Average RMSE
LR	0.83	0.080
MPR (degree 2)	0.96	0.030
DTR	0.86	0.070
RFR	0.89	0.060
SVR	0.87	0.068
XGBoost	0.98	0.029
MLP	0.98	0.029

K-fold CV is also a powerful statistical technique to assess the accuracy of ML models. This technique is particularly useful when the dataset is small, as it allows for a more accurate estimation of the accuracy of the model. Furthermore, when compared to other approaches such as the holdout CV, the k-fold CV is anticipated to show more robustness to the data set size [154]. Therefore, average R^2 and RMSE for four folds of k-fold CV were considered to evaluate the models' performance. This mean result is anticipated to reflect a more accurate estimate of the true unknown underlying mean performance of the model on the dataset, as computed using the standard error. Table 6 depicts the performance results of the various ML models employed in this study.

Similar to traditional statistical analysis, an ML model which maximizes R^2 and minimizes RMSE is deemed more accurate. Looking at the results, all models have performed better than the LR baseline model. The performance of the DTR, RFR, and SVR was almost identical with DTR exhibiting the weakest performance. This might be attributed to the fact that the DTs' performance degrades when it comes to intricate interactions between the features. DTs have a tendency to be a simpler model compared to RFR and SVR. DTs can struggle to capture complex relationships in the data. DTs also suffer with the change in data and exhibits a myopic behavior. During the fragmentation process in DTs, the overall insight on view of the data also reduces [155]. The results also suggest that RFR performed better than DTR. This might be attributed to the "bagging" effect. By aggregating multiple DTs, RF reduces biases and errors, resulting in more accurate environmental impacts predictions. Since each tree is trained on a random subset of the data, the impact of noisy data points is also reduced. The averaging of multiple trees also helps smooth out the effect of noise, resulting in improved performance compared to individual DT [156–158]. The better performance of SVR in comparison to DTs might be attributed to its ability to handle high-dimensional datasets, which is often a characteristic of AM's environmental impact prediction tasks. SVR achieves this by utilizing an optimized sample for support vector calculation as well as hyperplane definition through prioritizing samples that lie on the edge of the class distribution in feature space, thus making it appropriate for use with high dimensional datasets [159]. By utilizing kernel functions to transform the data into a higher-dimensional feature space, SVR can also capture the intricate patterns and non-linear dependencies present in AM data. This is in contrast to DTs, which may struggle to adequately represent such non-linear relationships performance [160]. However, SVR depends on the distance between various observations. If

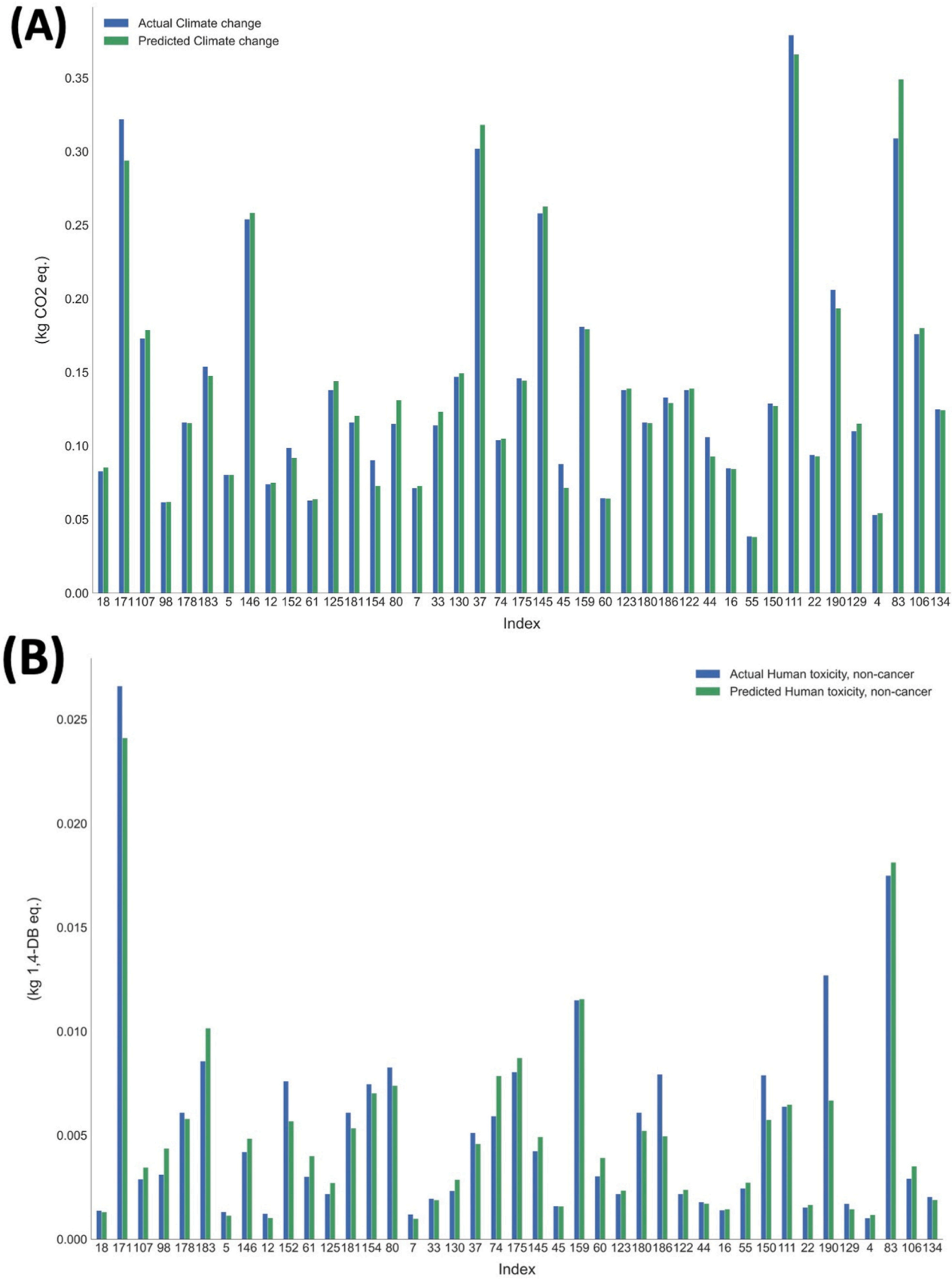

Fig. 10. Actual vs. (A) XGBoost predicted climate change, and (B) MLP predicted human toxicity noncancer. Note: The x-axis represents the index of the testing data, with each index corresponding to a specific data point within the testing dataset.

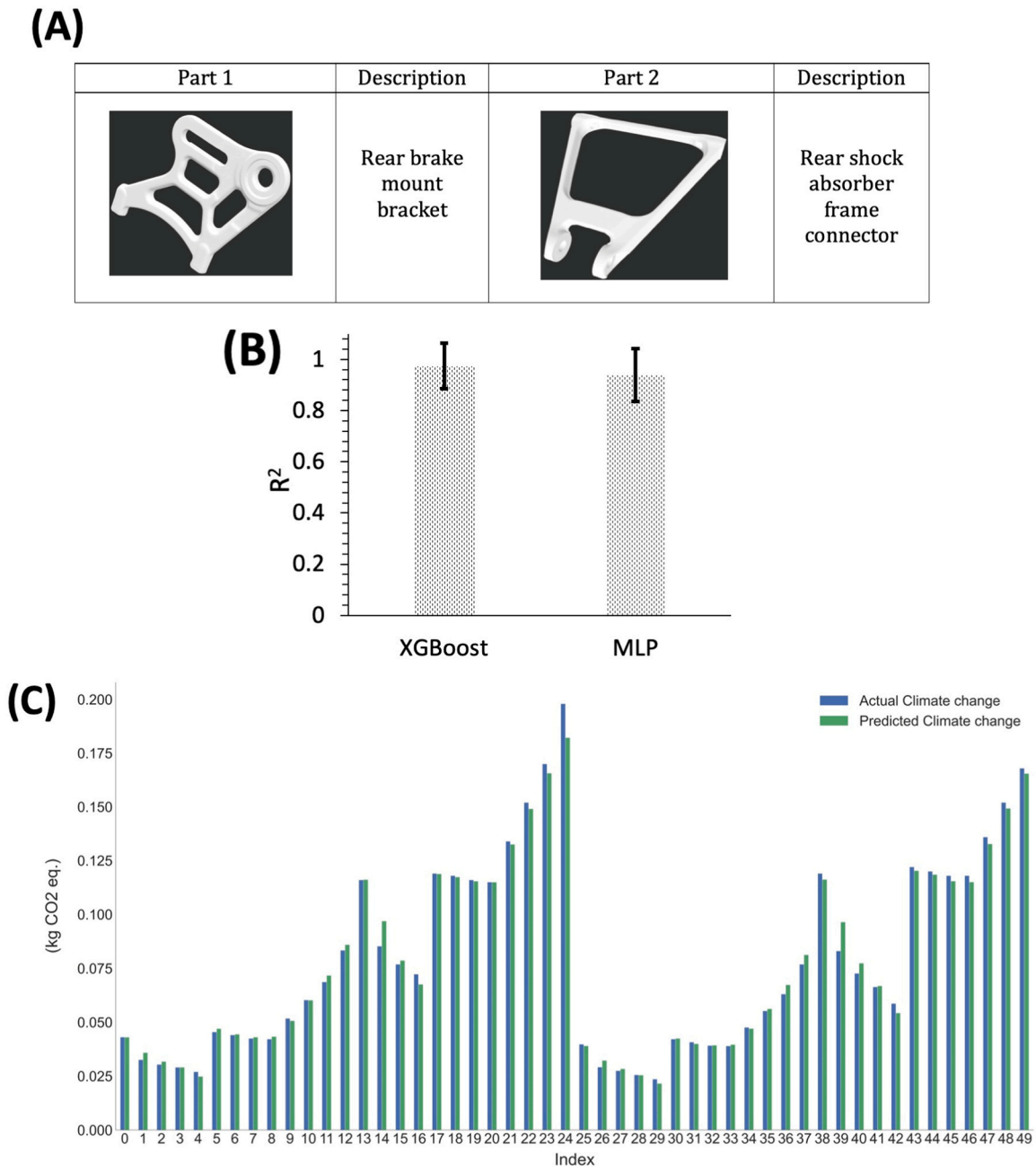

Fig. 11. (A) The two CAD files used for validation, (B) Average R^2 values for MLP and XGBoost on the validation dataset (Note: Error bars represent the standard deviation), and (C) Actual Vs. MLP predicted climate change (Note: The x-axis represents the index of the validation data, with each index corresponding to a specific data point within the validation dataset).

the value ranges of various flows differ greatly, the distance becomes less meaningful which then may explain the poor model performance in comparison to XGBoost and MLP [161].

Both XGBoost and MLP outperformed all the other models. XGBoost constructs an ensemble of weak prediction models (usually DTs) sequentially, where each subsequent model corrects the errors made by the previous models. In the case of AM, where various factors contribute to the environmental impacts, this iterative process allows XGBoost to capture complex patterns and interactions in the AM data, potentially leading to improved performance compared to other models. XGBoost also provides various regularization techniques, such as control over tree complexity, shrinkage (learning rate), and subsampling of data instances and features. These regularization methods help enhance the generalization capability of the model. By carefully tuning these parameters, XGBoost can optimize the trade-off between bias and variance, which may have contributed to its better environmental impact predictions [141,162,163]. On the other hand, the high performance of MLP might be attributed to its capability of learning hierarchical representations from the AM data. Environmental impacts of AM can arise from a combination of various factors such as energy consumption and interactive relationships between design-process parameters. These relationships can be highly non-linear and intricate. MLP's architecture, consisting of interconnected layers of nodes, allows it to capture and represent these complex non-linear dependencies accurately. Further, MLP has the ability to learn and model complex non-linear relationships as well as to generalize and infer hidden relationships on unseen data. In addition to that, MLP does not impose any restrictions on the feature variables and their distribution [156,164]. Compared to XGBoost and

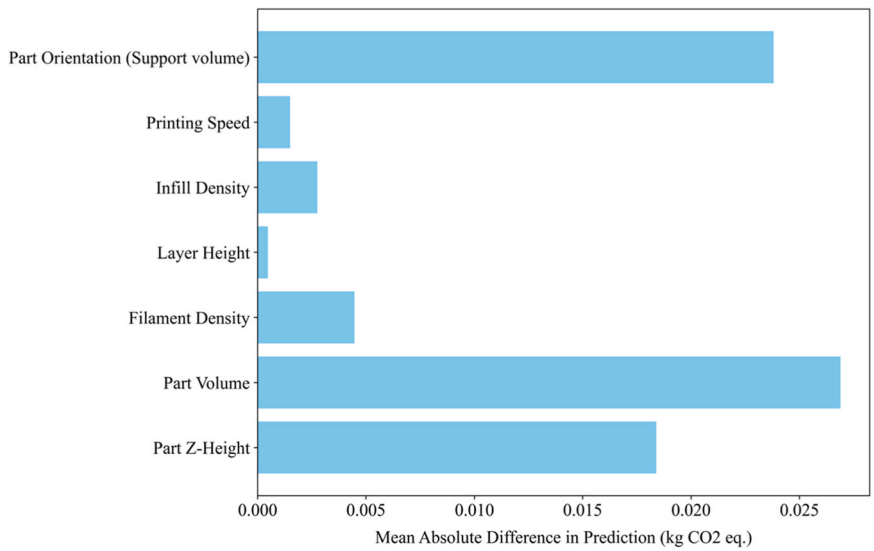

Fig. 12. Sensitivity analysis for the climate change impact category.

MLP, degree two MPR reflected a slightly lower prediction accuracy. Nonetheless, for high-dimensional problems, MPR becomes impractical due to its prohibitive number of product terms [137]. As the number of variables or features in the regression model grows, the number of possible combinations of terms increases significantly making the MPR unviable to employ.

These findings suggest that XGBoost and MLP are well-suited for the dataset of this research investigation due to their high accuracies and minimal overfitting tendencies, while DTRs and RFR could benefit from more data to improve their performance. Thus, we recommend predicting the environmental impacts of the FFF process using XGBoost and MLP. This facilitates the use of both of these models in parallel and aids in investigating cases where these models yield similar conclusions and/or can complement each other in out-of-sample case studies. Fig. 10 (A) depicts actual versus predicted XGBoost results for the climate change environmental impact criteria while Fig. 10 (B) shows predicted MLP results for the human toxicity-noncancer impact criteria. Results for the other impact categories were generated in a similar manner. Actual versus predicted MLP results for the other environmental impact categories are provided in the supplementary material section.

5.3. Model generalizability

In order to assess the model's generalizability and evaluate its performance on unseen data, we have tested the DD-LCA model using two CAD files [123] that were not included in the model's training dataset. For this purpose, a separate validation dataset consisting of 50 distinct data entries was utilized. The validation dataset was then fed into the trained model, and the corresponding environmental impact predictions were generated. Fig. 11 (A) depicts the two CAD files used for validation while Fig. 11 (B) shows the average R^2 values obtained from applying XGBoost and MLP models on the validation dataset. The high R^2 values obtained for both the XGBoost and MLP models indicate a strong level of generalizability. This suggests that the models have effectively learned from the training data and can successfully apply that knowledge to unseen CAD files, highlighting the reliability of both these models in predicting AM's environmental impacts. Fig. 11 (C) depicts actual versus MLP predicted results for the climate change environmental impact criteria for the validation dataset.

5.4. Sensitivity analysis

Another advantage of utilizing the DD-LCA model is the ability to promptly identify "hotspots", critical parameters that have a pronounced effect on AM's environmental impacts. Identifying these parameters provides decision-makers with insights into which aspects of the manufacturing process can be optimized to achieve better environmental outcomes. Essentially, these hotspots highlight areas in the AM process that, when adjusted, can lead to a more environmentally benign production. One effective strategy for identifying these "hotspots" is the application of sensitivity analysis. Sensitivity analysis provides a systematic examination of how different values of an independent variable (input parameter) can influence a particular dependent variable (output) while keeping other input parameters unchanged. Thus, a sensitivity analysis study was conducted to determine how alterations in the input parameters can influence the environmental impacts. The steps are as follows:

1. Perturbation of input data: Each input parameter was increased in value by 10%, while all other inputs remained unchanged, producing a set of perturbed data.
2. Prediction with original and perturbed Data: The trained XGBoost model was then utilized to predict outcomes of both the original and the perturbed data.
3. Calculation of mean absolute difference: The predictions derived from the original and perturbed data sets were compared, leading to the calculation of the mean absolute difference in predictions. This metric represents how much the prediction changes when tweaking a specific parameter by 10%. If changing an input causes a big shift in the prediction, then it is likely that this input will be a potential hotspot.

Fig. 12 depicts sensitivity analysis results for the climate change impact category. Results suggest that part volume, part orientation (represented by support volume), and part Z-height are potential hotspots. A careful control of these parameters is anticipated to yield a reduction in the climate change impact category. Table 7 summarizes the hotspots for each of the environmental impact categories, ranked in order of significance from 1 to 3 (where applicable), where 1 represents the most critical hotspot for each category. This approach provides a roadmap for designers and decision-makers, recommending where tweaks and optimizations can render the most ecologically beneficial results.

Table 7
Summary of the identified hotspots for each impact category.

LCA Impact category	Hotspot/s
Climate change	1. Part volume. 2. Part orientation (support volume). 3. Part Z-height.
Fine particulate matter formation	1. Filament density. 2. Part volume. 3. Part orientation (support volume).
Fossil resource scarcity	1. Filament density. 2. Part orientation (support volume). 3. Part volume.
Water use	1. Part volume. 2. Part orientation (support volume). 3. Part Z-height.
Freshwater ecotoxicity	-Filament density.
Freshwater eutrophication	-Filament density.
Human toxicity: cancer	1. Part volume. 2. Part orientation (support volume).
Human toxicity: non-cancer	-Filament density.
Ionizing radiation	-Filament density.
Land use	-Filament density.
Marine ecotoxicity	-Filament density.
Marine eutrophication	-Filament density.
Mineral resource scarcity	1. Part volume. 2. Filament density. 3. Part orientation (support volume).
Photochemical oxidant formation: terrestrial ecosystems	1. Filament density. 2. Part volume. 3. Part orientation (support volume).
Photochemical oxidant formation: human health	1. Filament density. 2. Part volume. 3. Part orientation (support volume).
Ozone depletion	1. Filament density. 2. Part volume. 3. Part orientation (support volume).
Terrestrial acidification	1. Filament density. 2. Part volume. 3. Part orientation (support volume).
Terrestrial ecotoxicity	1. Filament density. 2. Part orientation (support volume).

6. Conclusions and future research directions

In the initial stages of AM process conceptualization, it is essential to gain insights into the environmental implications associated with the design and process. Acquiring such insights enables the implementation of proactive measures to mitigate any potential adverse effects. The conventional data-intensive LCA procedure may encounter inefficiencies in the early stages of AM process design, especially when significant background and foreground inventory data are still unavailable. Thus, there is a need for a proactive and easy approach, specifically tailored for additively manufactured parts, that helps avoid the expenses associated with addressing environmentally unfavorable solutions in later design phases or retrofitting initiatives. At the same time, the integration of ML into LCA has demonstrated remarkable effectiveness in accurately predicting the environmental impacts of applications outside the AM domain. Thus, this paper has presented a potential solution by introducing an automated tool for LCA of AM that leverages the fruitful integration between ML and the product process co-design concept. The proposed approach was illustrated by taking the FFF process as a case study. Out of all the various ML models evaluated in this study, XGBoost, and MLP were found to be particularly effective in generating highly accurate predictions with a prediction accuracy of 98%. To validate the performance of these two models, a separate validation dataset comprising 50 unique data entries was employed. This dataset corresponded to two CAD files that were not included in the training process, ensuring that the evaluation was conducted on previously unseen data. Results showed that both models exhibited a good capability for generalization. Sensitivity analysis was also performed to identify environmental hotspots and offer guidance to designers and decision-makers, recommending areas where adjustments and improvements can yield the greatest ecological advantages. While this method deviates from conventional LCA approaches and requires further testing and discussion, it presents a highly promising and straightforward means of promptly and accurately predicting the environmental impacts of additively manufactured parts prior to printing. The proposed tool provides a viable substitute for conventional LCA approaches, offering AM practitioners a solution that reduces the need for extensive knowledge of LCA and its interpretations. This streamlined approach alleviates the challenges associated with the classical environmental impact assessment methods, providing a more accessible and efficient solution. With appropriate modifications, the proposed approach has the potential to be applied to various AM technologies. The findings from this analysis lay the foundation for subsequent modeling and predictive analysis, supporting the development of robust, data-driven, and ML-based approaches for assessing the environmental performance of AM.

Yet, it is important to acknowledge the various limitations of the current study. One limitation is related to the number of parts used to build the training dataset. The limited number of parts may affect the generalizability and representativeness of the results. A further limitation is associated with the number of data points available in the dataset. Thus, several promising research directions can be explored to pave the way for future advancements and broaden the scope of research in this field. One potential research direction for future investigation is to expand the training dataset by automating the feature extraction process. This can be done by developing standardized data extraction algorithms for AM parts and processes that are capable of utilizing computational power to rapidly extract AM features (e.g., support volume) with a commonly acceptable degree of error. Another future research direction may involve investigating the environmental implications associated with AM features that have been less explored in the literature (e.g., base area, cross-sectional area, and air gap). Another potential research direction can entail including more AM design and process features in the preliminary list of influential features. Another interesting avenue for future research can include examining the adaptability of the proposed methodology to other areas within the context of AM (e.g., composite AM and Big-area AM (BAAM)). For instance, it can be interesting to investigate whether the fiber material type and fiber orientation can exert a substantial influence on AM's environmental impacts. Another intriguing area of future research could involve developing ML-assisted consequential LCA. Developing an automated consequential LCA could provide significant support to decision-makers, offering a novel way to assess the environmental impacts in real-time or with more dynamic parameters. Specifically, if a manufacturer is considering introducing a new product to the market, an ML-assisted consequential LCA model could promptly provide insights into the potential environmental implications. An additional prospective research direction could involve developing automated tools for AM's social and economic LCA. Further research, including comparative and in-depth single case studies, is still needed to gain a more comprehensive understanding of AM's environmental implications and develop efficient assessment methods.

Declaration of competing interest

The authors declare that they have no known competing financial

interests or personal relationships that could have appeared to influence the work reported in this paper.

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Appendix A. Supporting information

Supplementary data associated with this article can be found in the online version at doi:10.1016/j.jmsy.2023.10.009.

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