Perspective│ Received 9 October 2024; Accepted 18 January 2025; Published 23 January 2025
https://doi.org/10.55092/aimat20250005

Machine learning modeling for material science and manufacturing: overview and perspectives for the future

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Highlights:

- Investigated the requirements for ML training and limitations compared to conventional modelling.
- Discussion of methodologies to improve the accuracy of ML beyond the latent space.

Abstract: It is undeniable that artificial intelligence (AI) and machine learning (ML) have become rooted at every level of our society. It is also true that engineers have always strived for improvement in design, materials, and manufacturing, the three cornerstones encapsulating most engineering challenges. Hence, it is no surprise that recent years saw a surge in engineering contributions employing AI and ML techniques. However, conversely to analytical models and finite element or finite volume analyses (FEA, FVA), and despite the countless pros, AI and ML models also present several cons. Trying to avoid a lengthy analysis of all discernable aspects, this perspective focuses on two specific prospects: one inward and one outward-oriented issue, each representing a weak point for ML approaches but also a challenge. On the one hand, ML models' formulations are well-known and documented. However, to achieve reasonable accuracy, the quality and size of the training dataset is paramount, making its definition as important as the architecture of the ML model itself. On the other hand, the prediction accuracy outside of the latent space, and how to improve it, remains a huge question mark, and often a limitation to more traditional yet reliable approaches, such as analytical, FEA, and FVA modeling. At this point, two questions arise. The former: what are the criteria to define whether ML has an edge over conventional modeling approaches? While the latter: how to design ML models capable of being less of a black box and better performing outside of the latent space? Each question is addressed separately in a section of the paper, together with a summary of the available state-of-the-art and a commentary of the authors' perspective on the matter.

Keywords: artificial intelligence; machine learning; material science; manufacturing; modelling; prediction; optimization.

1. Introduction

The integration of ML techniques into material science and manufacturing is revolutionizing these domains by enhancing production capabilities and enabling the intelligent management of complex data systems. Since the end of the 1990s, emphasis has been placed on hybrid approaches that combine human and machine intelligence to address real-time, uncertainty-laden challenges in manufacturing [1]. In the following years, this trend kept expanding and showed unprecedented growth in ML modeling techniques, as well as their role in addressing key industry challenges such as process optimization, cost reduction, and quality management [2]. Moreover, due to its nature, ML research is inherently multidisciplinary and interdisciplinary, creating possibilities for collaboration and exchanging ideas [2–4].

From a global perspective, ML applications can be divided into several categories, such as the type of task they solve (supervised, unsupervised or reinforcement learning), the type of model architecture (neural networks, ensemble models or kernel-based methods) and the application domain. To limit the focus of this paper, the application domain of interest will be material science and manufacturing and will be discussed in detail.

Over the last few years, ML has been used as a tool in the analysis and optimization of the material science and manufacturing engineering fields of metallic materials [5–7], polymeric composite materials [8,9], and recently, the AM processes [10,11]. Nevertheless, the problem of how to collect enough high-quality data to adequately capture the engineering problems remains the major concern [12].

The application of ML in manufacturing engineering is vast and it encompasses processes such as process optimization, scheduling, quality and maintenance [13]. For instance, in reference [14], deep reinforcement learning has been employed to minimize the delays in the workshop scheduling. ML methods have also been used in the process parameters optimization, for example in fused filament Fabrication to increase tensile strength with the help of Taguchi experimental design [18] and injection molding to minimize the product weight [19].

In material science, the gradient boosting algorithm was applied to predict flow stress of high-entropy alloys and the results showed that the proposed model performed better than conventional models [20]. Similarly, ML models have been found to be efficient in estimating the flow stress of the aluminum alloys under dynamic strain aging [21] and simulation of stress-strain curves for thermoplastic polymers with higher accuracy than phenomenological models [22]. In addition, surrogate models have been used to represent magnetic characteristics in terms of direction and microstructure [23].

In addition to the applications discussed so far, machine learning methods themselves are continuously evolving, unlocking new possibilities. In this regard, transfer learning is considered an enabler, allowing the use of other data sources if no sufficient ML database is available or data shifts are observed in comparison to the original training latent space [24]. The transfer task itself can differ, but common settings in manufacturing refer to a mapping between different working conditions (domain shift), between different machines or processes, or from simulations to real-world (experimental or production) data [25]. For instance, in additive manufacturing, [26] conducted a transfer between the FFF and selective laser melting for quality prediction and reference [27] investigated the domain shift within the FFF under different working conditions. To this end, in metal forming, the feasibility of transfer from synthetic ring rolling data, as well as the transfer between different mills, has been explored [28].

On top of that, recent advances in ML modeling saw the introduction of Physics-Informed Neural Networks (PINNs), representing a sort of bridge between traditional modeling approaches and ML, trying to address the issues of prediction accuracy and performance outside of the latent space [29]. Though revolutionary, PINNs are based on the implicit assumption of the availability of physical laws on which to base the update through backpropagation, limiting their utilization in areas such as manufacturing engineering [30].

Regardless of the application field or architecture, ML models require well-structured data for proper and reliable training [31]. This is particularly the case for manufacturing engineering, where data are collected and stored but are frequently unstructured, noisy, or incomplete, leading to challenges in applying ML techniques effectively in classification, clustering, and regression tasks. Raw data from machine sensors and manufacturing environments can also be filtered and then stored, reducing the amount of information extractable during the training process, as documented in the case of the radial-axial ring rolling process [32]. However, as also advised in this contribution, the storing of the raw data is advised to cope with possible issues of the filtered data and the relevant loss of information.

In general terms, regardless of source of the data for the construction of the training dataset, structured databases are complex to design and expensive to create [33]. The issue of data pre-processing and/or generation for the definition of the training dataset in ML is transversal across disciplines and is especially the case for materials science and manufacturing engineering, where complex experiments or lengthy FEA/FVM simulations need to be carried out to generate the training database [34–36].

Summarizing, in recent literature, the two key aspects related to the quality of the training dataset and extrapolation capabilities of machine learning have been lengthy discussed but still represent one of the key issues for a more widespread and efficient utilization of ML in material science and manufacturing. To this end, this perspective aims at providing an insight into the following two aspects:

What are the key aspects worth considering when choosing traditional approaches, such as analytical models, FEA, FVM, *etc.*, rather than creating an *ad-hoc* training dataset to train a ML model?

What are the available options to improve the extrapolation capabilities of ML models outside of the latent space to improve their application range and longevity?

To better understand the overall organization of this perspective, Figure 1 provides a comprehensive summary of the current state-of-the-art in machine learning (ML) for material science and manufacturing engineering considering the category of the modeling approach, the application field withing the scope of this perspective paper, and the recent developments, in terms of improved modeling approaches employes in these two fields of research. In the same diagram, the two above-mentioned questions are also reported and link to the various challenges facing ML applications in the research fields considered in this perspective. The path forward, as envisioned in this perspective, involves improvements in planning of the modelling approach, in the reducing of preprocessing time, as well as in the extensive usage of external knowledge in support of the conventional training dataset to reduce the amount of labeled data required for an effective training.

Ultimately, the aim of this perspective is to provide an insight into the current challenges facing ML applications, with special attention to the material science and manufacturing engineering fields, while also providing the authors’ vision for the steps required to improve the current state of the art and bolster effectiveness and longevity of ML models regardless of the field of application.

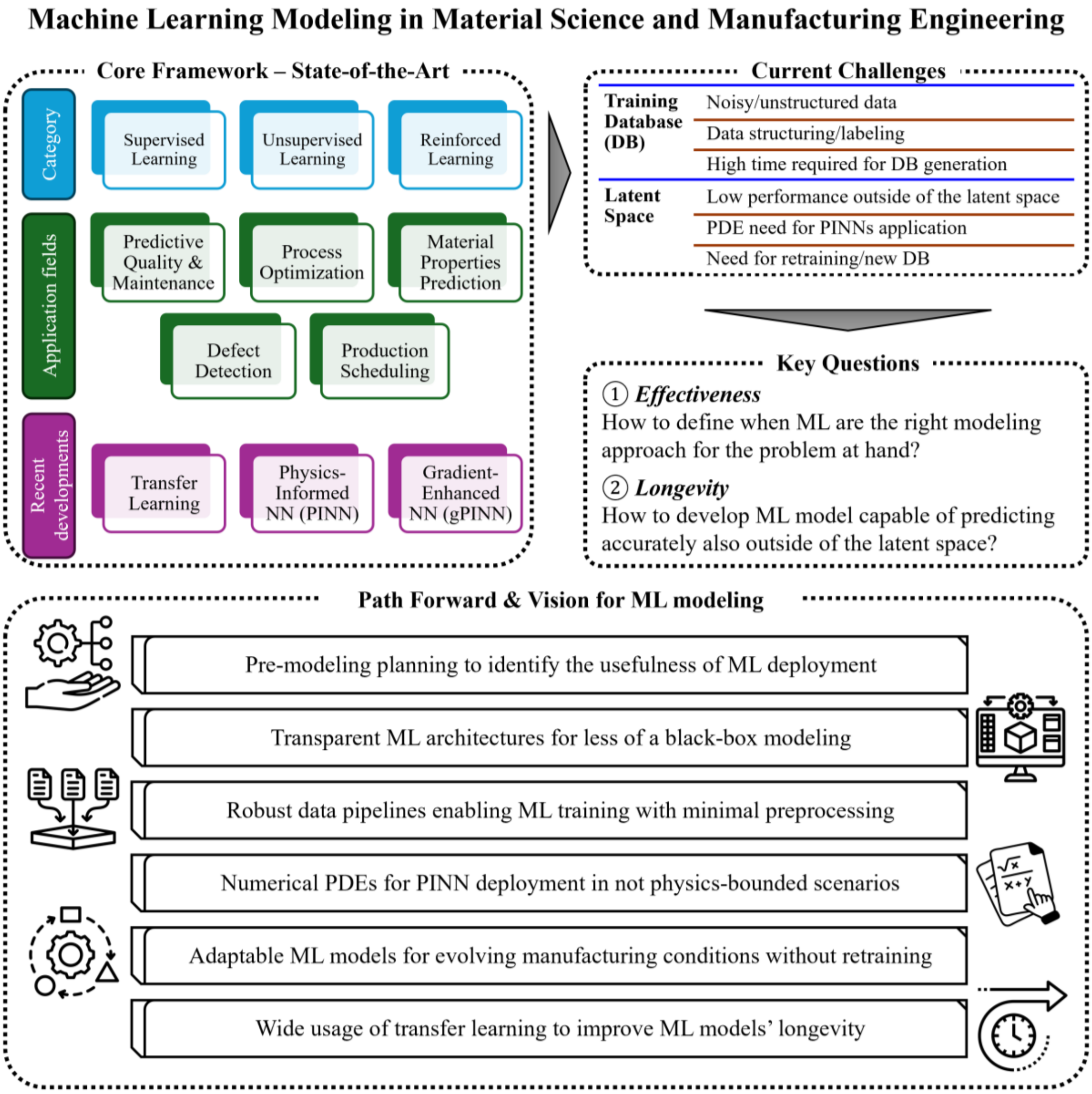

Figure 1. Summary of the current state-of-the-art, challenges, key questions, and envisioned path forward for machine learning models development and utilization in material science and manufacturing engineering-related tasks. This figure includes icons by multiple authors from Flaticon.com.

2. Does ML have an edge over conventional approaches?

This first question is, by definition, provocative and aims to stimulate fruitful pondering over the pros and cons of ML modeling. To contextualize, for more than 50 years FEA and FVM simulations represented the most trusted and utilized approach for engineering modeling and problem solving [30]. However, in recent years, we witnessed a spike in the interest in ML solutions to address engineering problems, resulting in a drastic increase in scientific publications [37]. However, is a ML model always better than an FEA/FVM simulation or even an analytical model? From the point of view of the authors of this perspective, the answer is no. As is well-known by everyone dealing with AI, the model is as good as the data employed to train it, meaning that the training dataset rather than the ML model, has far more far-reaching consequences on the quality of the predictions [38,39].

Since ML models learn patterns within their latent space, the question of data gathering, generation, and especially quality, and their influence on result reliability, especially with respect to unseen data, should be considered. Like conventional modeling approaches, which follow physically bounded rules, ML models can show a deterministic behavior too, but their accuracy can only be tested on discrete samples, *id est* test data. However, test data can never reflect all circumstances of the modeled distribution since they are limited by their boundaries.

In this regard, an interesting example is provided in reference [40] where the issue of labeling for sparse datasets from industrial environments and the need for the generation of benchmark results are key issues in the field of predictive quality in industrial environments.

To this end, the focus should be oriented towards designing the training dataset to be effective for the task at hand while considering the time required to do so. It is also worth pointing out that the response from more traditional approaches, such as analytical models, is direct, meaning that the model complexity is fixed. Similarly, FEA/FVM modeling is based on the considered scenario and relevant boundary conditions and yields variable precision as a compromise with the computational time.

However, in the case of ML models, the real challenge is to define the number and distribution of data points required for an effective training beforehand. This fact makes the training database design an optimization task of its own with a direct influence on training data quality [39], subsequently propagated to model selection, hyperparameters tuning, prediction accuracy, and so on. In this regard, the database generation requires feature planning [41] to select and include only the most influential ones and avoid data noise. A promising solution to reduce the time required for database generation is represented by a hybrid approach including both simulations and/or experimental observations and structured synthetic data [42]. Such hybrid databases, generated by merging different data sources, aim at data quality and information density rather than mere data point quantity.

Same concerning training database generation, although the collection of experimental and industrial data represents a viable solution, the sparseness of raw data, format differences, and consolidation strategies still represent a challenge [40]. In this regard, techniques such as domain adaptation and transfer learning offer a compromise to enhance the longevity of machine learning models, as successfully demonstrated in reference [25] for the cases of predictive maintenance. Transfer learning allows for reducing the need for new data generation for model retraining and is also effective in extending the longevity of a trained machine learning model. However, while the meaningfulness of the collected data and the correlation with the intended target variables must be verified beforehand, diversity and randomness to avoid bias in the raw data should be ensured and showed to grant enhanced versatility and generality of the trained ML model, also for the case of large language models (LLMs) [43]. In light of what is summarized so far, the trend in the scientific community is towards the generation of high-quality databases [38,39,41], including various sources [40], up to synthetically generated samples [42], to maximize information density while minimizing the labeling and pre-processing time.

As a final remark, it should be noted that, while machine learning (ML) offers significant advantages in dealing with large datasets, identifying complex patterns, and providing predictive capabilities, its effectiveness is highly context dependent. In particular, ML may not always be the optimal solution for engineering problems where the training dataset must be generated from scratch using resource-intensive methods, such as FEA or FVM simulations. In this regard, the *ad-hoc* generation of a training database can result in prohibitive time and computational costs, which may outweigh the benefits of implementing an ML model. Consequently, conventional approaches might remain more practical and efficient for certain applications, such as highly customized scenarios where no generalization can be achieved. In other words, traditional approaches are more effective for targeted analyses, where a high level of detail in the results is desired for a single component, materials, or manufacturing process. Conversely, when generalization is achievable and the goal involves multiple investigations of similar components or processes, machine learning models should be the tool of choice. By doing so, the trained ML modeling can help reduce the setup effort and computational time associated with numerical simulations, such as FEM and FVM. All this highlights the importance of carefully evaluating the trade-offs between ML and traditional methods in terms of data availability, problem complexity, and computational feasibility before selecting a solution.

Hence, the answer to the initial question is neither straightforward nor obvious. However, it is crucial to consider this question at the outset of any new endeavor to avoid investing time and resources in database generation and model training when simpler, yet equally effective approaches could deliver similar results more efficiently.

3. Beyond training and towards a thoughtful ML

The second issue worth bringing forward is most likely the most important for any engineer dealing with prediction and optimization tasks. In a nutshell, the question that all AI developers, ML users, and even enthusiasts so often deal with is “Can machine learning learn pattern of unseen data, extrapolating new patterns in a similar way that humans do?” Apart from the philosophical aura of the question itself, from an engineering perspective, it requires a deep understanding of what we expect our trained ML models to do, which is far from a trivial question.

Currently available ML formulations cannot replicate the human learning processes, especially the ability to generalize knowledge beyond predefined data boundaries. However, advancements such as Physics-Informed Neural Networks (PINNs) and gradient-enhanced PINNs (gPINNs) demonstrate that embedding generalizable knowledge into ML models can partially bridge this gap. In other words, humans leverage on intuition, experience, and pattern recognition even from sparse and incomplete data, whereas ML models are bound by the data provided during training, excelling in interpolation but struggling with extrapolation unless additional guidelines, such as physics-based or user-defined rules, are provided.

From an engineering standpoint, it is well known that identifying the global *minima* or *maxima* is the goal of many engineering tasks, such as weight minimization, stiffness maximization, and so forth. An example of ML application for optimization tasks is provided in [18], where an Artificial Neural Network (ANN) was employed for process parameters optimization in the additive manufacturing process or the control optimization of a counter-rotating hoop stabilizer [44].

However, setting up an optimization task requires engineers to define the range of the features, or input variables, for the problem at hand, a fact that makes the identified “best point” to represent a global *minima* or *maxima* only in the considered variables ranges rather than an all-encompassing global and definitive answer. Indeed, also in ML modeling, the training dataset, and its performance are linked to the ranges of both features and target variables, making it exceptionally good in interpolation within the latent space and less predictable in extrapolation tasks [45]. Some work in the performance of machine learning models outside of their training space was done in the last year (2024) and showed promising results in terms of advanced Graph Neural Network (GNN) formulations for materials property prediction [46] and domain generalization through meta-learning, where knowledge is transferred across various tasks removing the need for retraining [47].

Reconnecting the previous paragraph, designing the training dataset implicitly means defining the model's interpolation and extrapolation boundaries, *id est* where the extent of the features and target variables' boundaries regression performances are inevitably going to change [38,39]. Rather than an issue, this fact is a consequence of the way ML learns, which is based on the training dataset that is provided. To address this issue, scholars successfully included physics, leading to the definitions of PINNs [29], which, in turn, requires physics-based PDEs to be operated. PINNs are particularly effective in the field of fluid mechanics where the well-established theoretical background relevant to the Navier-Stokes PDEs allowed for accurate predictions both within and outside the latent space for velocity flow fields, especially for complex turbulent flows [48]. Another recent work showed that, for PINNs, the number of hyperparameters and their tuning is secondary to the definition of the PDEs frame and the inclusion of second-order PDEs [49]. In other words, features selection and the robust PDEs problem definition are essential to achieve good performance and cannot be amended by hyperparameters tuning, as it is sometimes the case for other ML formulations, such as kernel, ensemble, and neural network (NN) models.

However, although promising and widely investigated, PINNs still require the definition of a set of governing PDEs to be employed as a sort of tuning frame at the exit of the neural network and before the backpropagation loop. An alternative to fully physics-bounded PDEs is represented by gradient-enhanced physics-informed neural networks (gPINNs), where derivatives of the output of the standard NN are employed to estimate the residuals, subsequently employed for the update of weights and biases during backpropagation. Recently, gPINNs were benchmarked against standard PINNs formulations showing improvements in forward and inverse problems, especially on small training datasets [50]. Considering its recent development, to the best of the authors' knowledge, the only documented engineering application for gPINNs is reported in reference [51] to predict rotor angles, frequency, inertia, and damping in power systems applications, but the modeling approach still resembles that of PINNs.

To the best of the authors knowledge, so far, gPINNs have only been employed together with physics-bounded rule to improve existing PINNs formulation, showing improvements in accuracy [50] and especially faster convergency [51]. However, if no physics-based PDEs are available, a viable option is represented by the definition of numerical-based PDEs translating engineering knowledge, experience, and know-how in rules to guide the ML during the training, enhancing the prediction accuracy and in extrapolation tasks.

In practical terms, the adaptation of the backpropagation branch of a NN to include numerical PDEs, resembling a gPINNs model, can be carried out by adding customized, or customizable, PDEs at the residual level before beginning the backpropagation. Though not physics-bound, if well set, the defined numerical PDEs retain all advantages of the gPINNs formulation and can be employed to learn from smaller databases, as well as improve prediction accuracy outside of the latent space. In practical terms, such modeling approach, defined by the authors of this perspective as expert-informed neural networks (EINNs), can be implemented by identifying first the most influential features in the database, defining then PDEs in the form of residuals representing the gradients of the output of the NN to the input features. Features selection is not mandatory but recommended to limit the computational complexity related to the numerical PDEs tuning phase. Cross-product PDEs should also be included in a sort of feature engineering at the residual level to account for the combined influence of a couple or triplets of features on the model loss, as also suggested by reference [49].

The hybrid modeling solution granted by custom-made PDEs, defined on the basis of user's prior knowledge of the problem at hand, allows for less of a black box approach and higher tuning of the ML model but also entails an equation discovery phase, with a relevant increase in the time needed for the model training. By converting engineering knowledge into PDEs and introducing them in the residuals' calculation of a NN, mimicking PINNs, might be a viable solution in creating a bridge across the training dataset boundaries, thus improving the domain generalization capabilities [49], ultimately resulting in more flexible ML models.

Indeed, the utilization of custom-made PDEs in a EINNs scheme brings forward the issue of how to translate knowledge into PDEs [50,52], meaning that the constraints put in place must reflect true boundaries or conditions related to the problem at hand, and not only create a bottleneck in the backpropagation structure. It is also true that increasing the complexity of the ML architecture and including more knowledge in the shape of user-defined numerical PDEs can expand the range of validity of the developed solution, but it also comes at the cost of higher computational time, especially in the form of equation discovery and its tuning.

In summary, while machine learning cannot replicate the intuitive and adaptive way humans learn, it is possible to guide ML models toward better generalization by embedding domain knowledge through physics-informed or expert-driven constraints. Approaches like PINNs and gPINNs are potential methods for enhancing the performance in extrapolation problems and reducing the "black box" nature of ML, thus making them more explainable. However, these approaches come with challenges, such as the reliance on accurately defined PDEs and increased computational complexity during training associated with the need for an equation discovery phase. In addition to that, even when PDEs are available, PINNs can still fail to model the phenomenon at hand, both within and outside the latent space as a consequence of a poor equation discovery phase, which still remains one of the most critical steps.

Ultimately, the key to advancing ML beyond the latent space lies in rethinking how we train models, incorporating not only data but also the principles and rules that govern the problem, which are normally independent of the latent space derived from the training dataset. By doing so, a better balance among flexibility, accuracy, and computational efficiency can be achieved, leading to a better and smarter deployment of ML models in material science and manufacturing engineering applications.

4. Summary and outlook

This paper provided a comprehensive state-of-the-art summary of key modeling approaches for machine learning (ML) model development in the fields of material science and manufacturing engineering, along with the authors' insights and perspectives. While offering significant potential, it should be noted that ML should be regarded as an additional tool in an engineer's toolbox rather than a universal replacement for traditional methods like analytical modeling or finite FEM/FVM simulations. A key aspect highlighted in this perspective is the critical importance of training database design and especially its boundaries, which is the most influential factor in ML modeling regardless of the application field, especially in terms of post-training performance. Besides, although the recent developments of new ML algorithms and the high interest of most of the research community, ML is not yet capable of fully substituting traditional engineering tools such as FEM/FVM or analytical models. In fact, for scenarios where a high degree of customization is required, ML might not be the right tool for the task, and it is the opinion of the authors that more traditional approaches should still be the option of choice. In this regard, ML should be applied judiciously to problems where generalization is achievable, for instance across similar components or processes, especially for the case of optimization tasks. Nevertheless, the role of ML is expected to expand significantly in the future, especially if the challenges related to (1) improving data quality, (2) enhancing extrapolation capabilities, and (3) integrating domain-specific knowledge are addressed and solved. By addressing these issues, ML can become a more versatile and reliable tool, also for the case of complex engineering problems. To do so, future research should focus on hybrid modeling architectures, transfer learning techniques, and the integration of physics-informed and expert-driven constraints to enhance the interpretability and generalization of ML models. Such advancements will not only bolster the efficacy of ML but also establish it as a trusted approach within the broader engineering toolbox. In conclusion, it is worth pointing out, that ML, like any modeling technique, should be selected based on its suitability for the problem at hand rather than being seen as a default solution. By continuing to address the current limitations and leveraging on its strengths, ML has the potential to foster growth and development in material science and manufacturing engineering and to coexist in a complementary manner with currently employed and reliable traditional approaches.

Acknowledgments

Prof. Luca Quagliato was supported by the RP-Grant 2024 of Ewha Womans University. The authors would also like to acknowledge the use of icons from multiple authors from Flaticon.com in Figure 1 and in the Graphical Abstract.

Conflicts of interests

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.

Authors' contribution

Conceptualization, L.Q., J.S., and M.P; methodology, L.Q., J.S., and M.P; investigation, L.Q., J.S., and M.P; resources, L.Q.; data curation, L.Q., J.S., and M.P; writing—original draft preparation, L.Q., J.S., and M.P; writing—review and editing, L.Q., J.S., and M.P; supervision, L.Q.; project administration, L.Q.; funding acquisition, L.Q. All authors have read and agreed to the published version of the manuscript.

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