MACHINE LEARNING EM MATERIAIS DENTÁRIOS RESTAURADORES

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RESUMO: Aprendizado de Máquina (do inglês *Machine Learning* - ML) é uma poderosa subárea da inteligência artificial que permite que os sistemas aprendam autonomamente com os dados e melhorem seu desempenho. As técnicas de ML são aplicadas em uma ampla gama de aplicações na área da saúde, como análise de imagens médicas, diagnóstico de doenças, planos de tratamento personalizados e desenvolvimento de medicamentos. Na odontologia, ML pode ser aplicado na previsão de propriedades de materiais dentários, com base em sua composição, estrutura e desempenho, o que pode levar ao desenvolvimento de materiais dentários restauradores mais seguros e eficazes. Este estudo realizou uma pesquisa abrangente de artigos usando bancos de dados respeitáveis e empregou vários termos de consulta relacionados a ML, odontologia e materiais odontológicos. Um total de 115 artigos foram selecionados de um pool inicial de 537 estudos, após análise e categorização. Esses artigos abrangiam várias especialidades odontológicas, sendo a implantodontia, a odontologia restauradora e a estomatologia as categorias mais proeminentes. Os artigos selecionados exploraram principalmente a viabilidade e precisão das previsões do modelo de ML, bem como comparações entre diferentes modelos de ML. Dentro da categoria de

odontologia restauradora, os modelos ML foram empregados para tarefas como design de coroas, identificação de materiais, previsão de cor e resistência para restaurações indiretas e avaliação do crescimento de biofilme. Uma variedade de metodologias de ML, incluindo regressão logística, redes neurais convolucionais e árvores de decisão de aumento de gradiente, foram empregadas nesses estudos. Embora o uso de modelos de ML na pesquisa odontológica tenha mostrado um crescimento notável, a aplicação específica de ML para o desenvolvimento e melhoria de materiais dentários restauradores permanece relativamente limitada. É fundamental reconhecer que os testes experimentais devem complementar os resultados obtidos dos modelos de ML para garantir sua confiabilidade e facilitar sua integração segura nas práticas odontológicas.
PALAVRAS-CHAVE: Machine Learning. Inteligência artificial. Odontologia. Materiais Dentários. Odontologia restauradora.

MACHINE LEARNING IN RESTORATIVE DENTAL MATERIALS

ABSTRACT: Machine learning (ML) is a powerful subset of artificial intelligence that enables systems to autonomously learn from data and improve their performance. In dentistry, ML might be applied in dental materials properties prediction, based on their composition, structure and performance, which might lead to safer and more effective restorative dental materials development. This study conducted a comprehensive article search using reputable databases and employed various query terms that relate to ML, dentistry, and dental materials. A total of 115 articles were selected from an initial pool of 537 studies, after analysis and categorization. These articles spanned various dental specialties, with implantology, restorative dentistry, and stomatology being the most prominent categories. The selected articles primarily explored the feasibility and accuracy of ML model predictions, as well as comparisons between different ML models. Image data played a significant role, with approximately 43.47% of the studies utilizing radiography, scanning electron microscopy, and photography. Within the restorative dentistry category, ML models were employed for tasks such as crown design, material identification, color and strength prediction for indirect restorations, and biofilm growth assessment. A range of ML methodologies, including logistic regression, convolutional neural networks, and gradient boosting decision trees, were employed in these studies. While the use of ML models in dental research has shown remarkable growth, the specific application of ML for the development and improvement of restorative dental materials remains relatively limited. It is crucial to acknowledge that experimental tests should complement the results obtained from ML models to ensure their reliability and facilitate their safe integration into dental practices.
KEYWORDS: Machine Learning. Artificial Intelligence. Dentistry. Dental Materials. Restorative Dentistry.

INTRODUCTION

Machine learning (ML) is a specific subfield of artificial intelligence that focuses on developing algorithms and models that allow systems to automatically learn and improve from data. Rather than being explicitly programmed to perform specific tasks, ML systems are designed to learn from data and extract useful information through patterns and relationships identified in the data. This allows them to predict, make decisions or perform tasks similar to what humans would do, based on previous examples.

The first ML studies date back to the 1950s and from the 2010s onwards, a great interest in this area began, with thousands of scientific publications on ML. ML encompasses various techniques such as supervised, unsupervised, reinforcement, and deep learning. These techniques have applications in many domains, which include image and speech recognition, natural language processing, recommender systems, fraud detection, and many others (Hastie et al. 2009; Goodfellow et al. 2016; Zhang et al. 2021).

ML has gained significant traction in healthcare, with several direct applications. Some of them include medical imaging analysis (X-rays, MRIs and CT scans) and diseases diagnosis and prognosis. Also, starting from genomic data, ML solutions already provide personalized healthcare predictions, treatment plans and also streamlines new drugs development, with greater predictability and precision. Health monitoring devices also utilize ML and monitor vital signs, sleep patterns and activity levels (Schleyer et al. 2006; Cirillo and Valencia 2019; Ngiam and Khor 2019; Schwendicke et al. 2020; Ahmed et al. 2021).

ML is also used for dental materials development, improving their properties, in terms of its composition, structure, and performance characteristics predictability, for example. They can predict material properties such as strength, hardness, biocompatibility, and wear resistance. It allows searching for the ideal composition or structure for new materials that meet specific criteria, such as mechanical resistance, aesthetic properties, or antimicrobial activity. They assess biocompatibility to develop materials that are safer and compatible with oral tissues, which reduces the risk of adverse reactions or complications (Schwendicke et al. 2020; Ahmed et al. 2021).

The aim of this study is to investigate the application of ML in Dentistry, with a focus on the development and improvement of restorative dental materials.

METHODOLOGY

This study was carried out based on a search in the PubMed, Scopus, and Embase databases, using the terms “machine learning”, “dentistry” and “dental material”, and their variations in different arrangements. Only scientific articles were included. There was no publishing date or language restriction. Retrieved data was tabulated in an Excel spreadsheet and analyzed. Articles were selected following PRISMA methodology guidelines (Page et al. 2021) (Figure 1). The inclusion criteria were: machine learning use, belonging to a specialty of Dentistry, and being related to either the development or improvement of a dental material, process, or procedure. The selected articles were organized into categories (Graphic 1). Then, these articles were used as input and a second inclusion criteria was applied, where only studies that addressed the development or improvement of restorative materials were selected. From these studies, data referring to the author, year of publication, study's aim and which ML model was used were extracted and analyzed (Table 1). The limitations of ML model applications were also addressed.

RESULTS

The initial query retrieved 537 studies. After duplicate removal and sorting, 115 (Figure 1) studies were organized into 8 categories: Endodontics, Implantology, Orthodontics, Periodontics, Public Health, Radiology, Restorative Dentistry, and Stomatology. Each of such categories' percentages are presented in Graphic 1. Implantology, Restorative Dentistry and Stomatology were the ones that had the highest production, with 30, 24 and 24 articles respectively.

In general, the studies investigated the feasibility and accuracy of model prediction and the comparison between models. The ML approaches used covered supervised and unsupervised models, neural networks, and deep learning. About 43.47% of the studies used imaging data. The use of images was observed in all categories. The most used images were radiography, scanning electron microscopy and photography.

Eight studies from the Restorative Dentistry category were included. About 87.5% (n=7) were published in the last three years. ML models were used to design lithium disilicate crowns, identify and differentiate restorative materials, predict color and strength of indirect restorations, and assess biofilm growth.

Logistic Regression methodologies associated with Maximum Likelihood (Chen, 2023), Trainable Weka Segmentation (TWS) plug-in (Ding 2022 and Vyas, 2016), 3D-DCGAN (Ding, 2023), Convolutional Neural Networks (CNNs) (Engels 2022 , Karatas, 2021), Regression Models (Kose, 2023), Extra Trees (ET) (Li, 2022), Gradient Boosting Decision Tree (GBDT) (Li, 2022), LightGBM (Li, 2022) and XGBoost (Extreme Gradient Boosting) (Li, 2022 and Vyas et al. 2016), Multilayer Perception (MLP) (Vyas et al. 2016) and K-Nearest Neighbors (KNN) (Vyas et al. 2016) of ML were applied in the selected studies (Table 1).

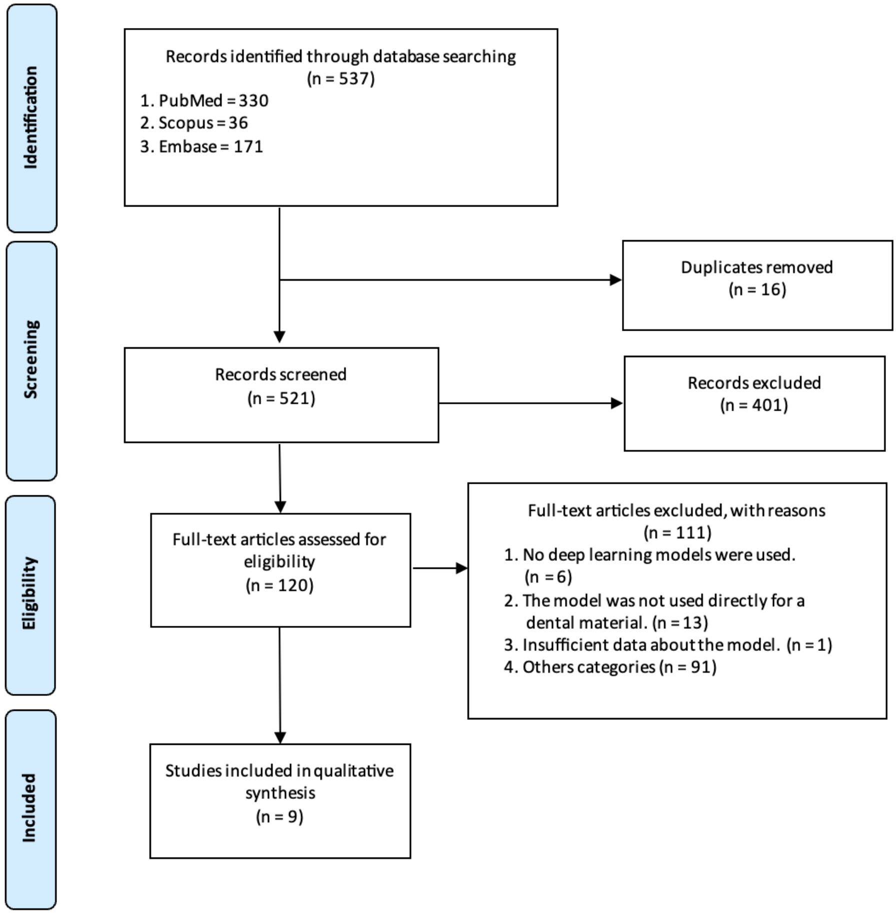
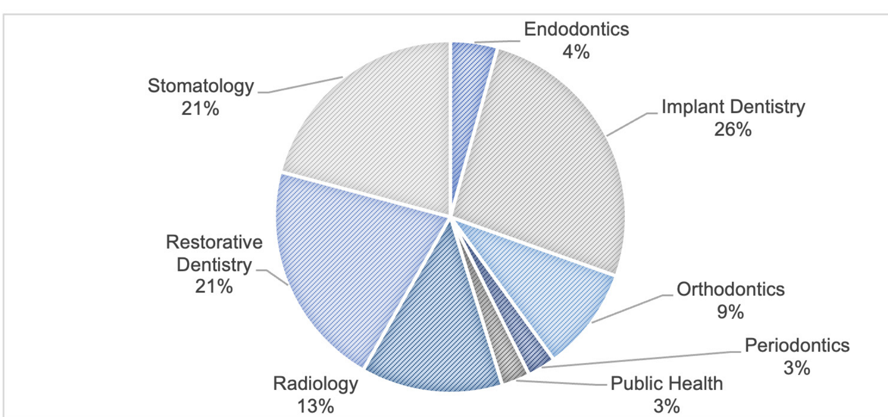


Figure 1: Methodology PRISMA Flowchart.



Graphic 1: Number (%) of studies that used machine learning according to dental specialty.

Author and Year	Aim of the Study	AI Application (ML Application)
Chen et al. 2023	develop a numerical probability value to identify dental compounds from mass spectrometry (MS) data.	An ML algorithm using logistic regression, optimized by the maximum likelihood estimation method.
Ding et al. 2022	to quantify initial bacterial adhesion on different dental materials using Scanning Electron Microscope (SEM) images.	Fuji Trainable Weka Segmentation (TWS) plug-in
Ding et al. 2023	development of designs for dental crowns in lithium disilicate	3D-DCGAN (a specific type of convolutional adversarial generative network (DCGAN) applied to three-dimensional data)
Engels et al. 2022	Detection and categorization of dental restorations in posterior teeth (composite resin, amalgam, gold, ceramic) using intraoral photographs; determine the accuracy of the ML method with expert judgment (reference standard).	Convolutional Neural Networks (CNNs)
Karatas et al. 2021	detect and differentiate amalgam, composite resin, and metal-ceramic restorations based on interproximal and periapical radiographs.	Convolutional Neural Networks (CNNs)
Kose et al. 2023	final color prediction of leucite-reinforced glass CAD/CAM veneer restorations based on substrate color, ceramic color, thickness, and translucency	Regression models (n=28) of supervised learning imported from the scikit-learn API (www.scikitlearn.org).
Li et al. 2022	development of predictive models of flexural strength of CAD/CAM ceramic blocks and composite resin	Extra Trees (ET), Gradient Boosting Decision Tree (GBDT), LightGBM, and XGBoost (Extreme Gradient Boosting)
Suryawanshi and Behera 2023	to test three ML models for the analysis of dental composite wear immersed in chewable tobacco solution	Multi-layer perception (MLP); Extreme gradient boosting (XGBoost); K-Nearest Neighbors (KNN)
Vyas et al. 2016	model development for an accurate assessment of biofilm growth and disruption on surfaces using scanning electron microscopy images.	Trainable Weka Segmentation (TWS) plug-in

Table 1: Characteristics of studies in the restorative dentistry category focusing on the development or improvement of materials or procedures.

DISCUSSION

Machine Learning models have been widely used in different dental specialties. In this study, the selected publications exclusively used linear models or complex models, or a combination of both, comparing the results between these models. In general, the models aims on calculating the chances of predicting events such as diagnosis and lesions of dental caries and periodontal disease, cancer, root fracture and apical lesions, alveolar bone loss, extractions, need for orthodontic treatment and determination of age and sex from characteristics of mineralized tissues.

The present study initially encompassed 537 articles, out of which 115 focused on various subjects within the domains of Endodontics, Implantology, Orthodontics, Periodontics, Public Health, Radiology, Restorative Dentistry, and Stomatology. The results analysis revealed that most of the studies (88.77%) were carried out in the last 5 years (2019 - 2023), showing an increasing trend in such. This trend was also observed by Kanangar et al. (2021) when investigating the developments, applications, and performance of artificial intelligence in dentistry. The use of ML and other methodologies involving Artificial Intelligence is promising, with results that seek to automate and streamline drugs and diseases diagnosis, as well as to develop and improve materials, procedures, and dental services, while streamlining and assigning security to data management (Schleyer et al. 2006; Schwendicke et al. 2020).

Despite the elevated number of published scientific articles that used ML in Dentistry, there are still few that refer to the dental materials development or improvement. In this study, 9 scientific articles applied ML to improve the production performance of indirect restorations, differentiate restorative materials under conditions like those found in a clinical environment, identify color variations in restorations and evaluate biofilm growth.

Data-related factors such as availability, accessibility, structure, and scope, and methodology-related factors such as reduced methodological rigor and development models have been considered as limiting factors for a wider ML application (Schwendicke et al. 2020).

It should be considered that the concerns with concrete and measurable benefits or advantages of the improvements that these methodologies can provide in the prevention and early diagnosis of diseases, in the relief of pain and discomfort - and therefore in the patient's comfort and quality of life and well-being - in the functional and aesthetic optimization and in the aid to decision making is associated with ethical issues and and patient's trust and relationship with the health professional.

Several methodologies were used in dental materials development or improvement studies. A proper selection of machine learning models is of utmost importance to achieve accurate results. Different modeling algorithms have specific characteristics that make them more suitable for different types of problems and datasets. Choosing the right model can lead to a better understanding of patterns and relationships in the data, as well as an increased ability to make predictions and make decisive decisions. In addition, the proper selection of models helps to avoid problems such as overfitting (excessive adjustment to the training data) or underfitting (lack of adequate adjustment to the data) (Hastie et al. 2009; Goodfellow et al. 2016; Zhang et al. 2021).

Choosing an ideal ML algorithm depends on several factors, such as the nature of the problem, the amount and quality of available data and specific data characteristics. There is no single algorithm that is best for all situations. Key ML methodologies include supervised learning, in which the model is trained on labeled data to perform instructions or classifications; unsupervised processing, which seeks to discover patterns and structures in unlabeled data; and reinforcement learning, where the model learns to act based on rewards and feedback from the environment (Hastie et al. 2009; Goodfellow et al. 2016). This makes the selection of the most suitable model one of the main factors for obtaining satisfactory results that meet the proposed objectives of studies that use ML.

Constraints on ML models are not specific to instrument, sample type, or data analysis software (Chen et al. 2023). In this study, the observed limitations associated with the quality of the models and data resulted in the need for adjustments for a better model performance. In studies such as that by Ding et al. (2022), who evaluated scanning electron microscopy images of bacterial biofilms stained with a revealing agent, accuracy can be improved by increasing the quality of the data. This happened by correcting the illuminated background using the "rolling ball" algorithm, subtracting the background, improving the contrast obtained by the revealing agent, as bacterial growth occurs non-uniformly, removing outliers and increasing the sharpness of the image. While in Ding (2023), the complex geometry of dental crowns, the degree of surface polishing, and possible microcracks affected the quality of Finite Element Analysis (FEA) data used in the ML methodology.

The performance of ML models can be evaluated using metrics such as Accuracy (measures the proportion of examples classified correctly in relation to the total number of examples), Precision (evaluates the proportion of examples classified as positive that are actually positive and is useful when the focus is on minimizing false positives), Recall (measures the proportion of positive examples that were correctly identified by the model and seeks to minimize false negatives.), F1-score (combines precision and recall in a single measure and seeks a balance between both) and the Confusion Matrix (shows the correct and incorrect classifications made by the model for each class) (Hastie et al. 2009; Zhang et al. 2021). Studies of dental specialties that used Artificial Intelligence methodologies obtained accuracy between 75% and 98% (Khanagar et al. 2021). In this study, accuracy ranged between 81% and 99.4%. However, basing decision-making exclusively on performance metrics such as accuracy in healthcare can lead to misleading and potentially dangerous mistakes. Low precision values may indicate that the model is not working correctly and therefore it is not reliable enough to support clinical decisions. In addition, there are other factors to be considered, such as the model sensitivity and specificity, which can have a significant impact on clinical applicability (Moons et al. 2014).

As important as selecting the most suitable ML model, some additional care is required to obtain accurate results. For a more adequate evaluation with ML tools, one could use a sufficiently large dataset that guarantees good representativeness, properly split the data for training and testing, use regularization to assign the level of complexity closest to what the model requires, and use cross-validation like k-fold to get a more robust evaluation. A combination of several strategies may be required, depending on the specific problem and dataset in question (Goodfellow et al. 2016; Zhang et al. 2021).

CONCLUSION

The application of ML models in dental studies has increased rapidly in recent years. Its importance lies in the search for solutions or improvements to complex issues and thus contributes to a more personalized patient-centered clinical treatment and for processes, products, techniques, and dental services to be more effective and efficient. So far, the scientific production that uses ML for restorative dental materials development and improvement is limited. ML can contribute to dental materials development, allowing the advancement and agility of processes, projects, and material optimization. It is important to emphasize that the results obtained by ML models or other Artificial Intelligence methodologies must be complemented with experimental tests, guaranteeing results and facilitating their safe use.

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