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## **Application of Machine Learning in Dentistry: Insights and Challenges**

### **-Supplementary Material-**

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## **Section 1 Principles of ML application in dentistry**

### **a. Data collection and preparation**

-Data Quality and Quantity: data collected from various sources including digital radiographs, cone-beam computed tomography (CBCT) scans, intraoral photographs, 3D models, patient medical records and clinical notes should be findable, accessible, interoperable and reusable to be used in ML models <sup>1</sup>.

-Data Preprocessing: raw dental data often needs to be cleaned, normalized and preprocessed to eliminate the noise and fill missing values, ensuring the uniformity. This step introduces data augmentation techniques to diversify the dataset and improve model generalization <sup>2,3</sup>.

-Data Labeling: The accuracy of the labels is essential for ML subsequent reliable use in the clinical setting, this involves annotating images (e.g., identifying areas of decay or lesions), categorizing diagnoses or labeling treatment outcomes based on experts' opinions or clinical records <sup>4</sup>.

### **b. Model selection and training**

-Algorithm selection: choosing the right ML algorithms that match the specific application in dentistry. Common algorithms are listed as follows:

1)Supervised learning: including decision trees <sup>5</sup>, SVMs <sup>6</sup> and neural networks <sup>7</sup> mainly used for diagnosis, prognosis and classification of dental conditions.

2)Unsupervised learning: including k-means clustering <sup>8</sup> and hierarchical clustering <sup>9</sup> techniques used for data segmentation such as grouping patients based on similar risk profiles or treatment needs.

3)Reinforcement learning: used for developing optimal treatment plans <sup>10</sup> or robotic-assisted surgeries <sup>11</sup>, where models are continuously adapted and improved by receiving feedback from patient responses or treatment effectiveness.

-Model training: feeding the ML model with labeled data to learn patterns, relationships and features associated with specific dental conditions or treatment outcomes.

-Feature engineering: selecting or deriving the most relevant features from the dataset to achieve accurate model predictions. This might involve identifying specific attributes from dental images or extracting significant clinical information from patient medical records <sup>12</sup>.

### **c. Model evaluation and validation**

-Performance metrics: to assess the accuracy and reliability of ML models, common metrics including accuracy, precision, sensitivity, F1-score and ROC-AUC (Receiver Operating Characteristic - Area Under the Curve) will help to evaluate the reliability and clinical utility of algorithms for identifying, diagnosing or predicting under certain dental conditions <sup>13</sup>.

-Cross-validation: techniques like K-fold cross-validation <sup>14-16</sup> are used to validate the model's performance across different subsets of the data.

- Bias and variation: regularization and hyperparameter tuning in managing the bias-variance tradeoff is to prevent model underfitting or overfitting help, so as to optimize model performance <sup>17</sup>.

#### **d. Integration and implementation**

-Workflow integration: integrating ML models into existing dental workflows could provide the complement of clinical practices without disruption (e.g. diagnostic imaging software for real-time decision support) <sup>18</sup>.

-User interface design: the output of ML models should be presented in a user-friendly manner so that dental specialists can interpret and act on the provided information more easily, such as indicating the concerned area from a radiograph or giving a treatment plan based on predicted outcomes.

#### **e. Continuous learning and adaptation:**

-Model retraining: As new data available input (e.g., new patient cases, updated guidelines), ML models should be periodically retrained to maintain their accuracy, relevance and consistency with up-to-date clinical knowledge and practices.

-Feedback loops: Incorporating feedback from clinicians and patients to refine and improve model performance. Continuous feedback helps in identifying errors, updating models and enhancing the practicality of ML tools in clinical settings.

#### **g. Clinical validation and approval:**

-Clinical trials and validation: Before deploying ML models in real-world dental settings, rigorous clinical validation must undergo under condition involving clinical trials, pilot studies or comparative studies with existing diagnostic methods to ensure safety, efficacy and reliability. <sup>19</sup>

-Data security and compliance with regulations: As dentists and researchers harness clinical data for ML modeling, adherence to relevant data protection regulations is imperative. Ensuring compliance

with laws such as GDPR <sup>20</sup>, HIPAA <sup>21</sup> or CCPA <sup>22</sup> is crucial to maintain confidentiality and keep sensitive information safe from unauthorized access.

**h. Interpretability and explainability <sup>23</sup>:**

-Model transparency: Interpretable models allow dentist to clearly understand how models reach the specific decisions especially in critical areas such as diagnosis and treatment planning.

-Explainable AI (XAI): aims to develop a suite of ML techniques so that can produce more explainable models while maintaining a high level of learning performance (e.g., prediction accuracy) <sup>24</sup>, particularly for deep learning models often considered as "black boxes", using pathway visualization or feature highlighting in a diagnosis.

**i. Patient-centric <sup>25</sup>care:**

-Personalization: to create ML-personalized treatment plans according to patient's individual data such as genetic information, medical history, lifestyle and specific dental conditions.

-Improving patient outcomes: the ultimate goal is to provide faster and more efficient care that directly enhance patient outcomes <sup>26</sup>.

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