31º ENCONTRO DE QUÍMICA DA REGIÃO SUL
A QUÍMICA COMO PROPULSORA DE NOVOS ECOSSISTEMAS DE INOVAÇÃO
19 A 21 DE NOVEMBRO
Campus Toledo
Unioeste

Área: ANA_____
(Inserir a sigla da seção científica para qual o resumo será submetido. Ex: ORG, BEA, CAT)

Application of Machine Learning Algorithms in the Classification and Quantification of GSR

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Palavras Chave: *Análise de Imagem; GSR; Machine Learning; Perícia Forense; Química Analítica.*

Highlights

The study integrates spectrophotometric analysis, digital image processing, and machine learning, establishing an innovative approach for the detection and quantification of gunshot residues (GSR). The bromopyrogallol red (BPR) reagent enabled clear visual differentiation of elements, with antimony producing a pink coloration and lead yielding a purple hue, thus providing a robust chromatic basis for forensic analysis. Processed images generated color descriptors such as Hue, Saturation, Red, and Blue, which emerged as key variables for training and optimizing machine learning models. Among the algorithms tested, Random Forest (RF) and XGBoost achieved the best performance, delivering near-perfect sample classification and high predictive accuracy for concentration levels ($R^2 > 0.90$). The methodology proved to be reliable, efficient, and highly applicable, positioning itself as a promising alternative for forensic chemistry and GSR analysis.

Resumo/Abstract

This work presents a methodology for the detection and quantification of gunshot residues (GSR), combining spectrophotometric analysis, digital image processing, and machine learning, with the objective of developing a robust and highly accurate system for forensic applications. The methodology begins with the complexation of samples using the Bromopyrogallol Red (BPR) reagent, which reacts selectively with antimony and lead, the main components of GSR [1]. This reaction produces distinct colored complexes (pink for antimony and purple for lead), serving as the visual basis for analysis. Images were captured and processed with the GIMP software to extract color descriptors such as Hue, Saturation, Red, and Blue. The Chemostat software was then used to convert the visual data into numerical information suitable for predictive modeling [2]. Several machine learning algorithms were tested and compared, with Random Forest and XGBoost standing out for their superior performance. In classification tasks, the models achieved an area under the curve (AUC) close to 1.00, indicating an almost perfect ability to distinguish GSR samples from non-shooting samples. In quantification, the coefficient of determination (R^2) exceeded 0.90, validating the precision of concentration estimates. Interactive model analysis confirmed the relevance of color descriptors in predictions, reinforcing the validity of the visual approach. In conclusion, this research establishes a reliable and promising method for forensic science, combining the sensitivity of a chemical reaction with the predictive power of machine learning, thus representing a significant advancement for forensic investigations and analytical chemistry.

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Agradecimentos/Acknowledgments

Universidade Estadual do Centro Oeste do Paraná - UNICENTRO, CAPES e 16º BPM de Guarapuava.