Simultaneous Dual-Analyte Detection Biosensor through Stacking-Based Ensemble Machine Learning Approach: Design and Optimization

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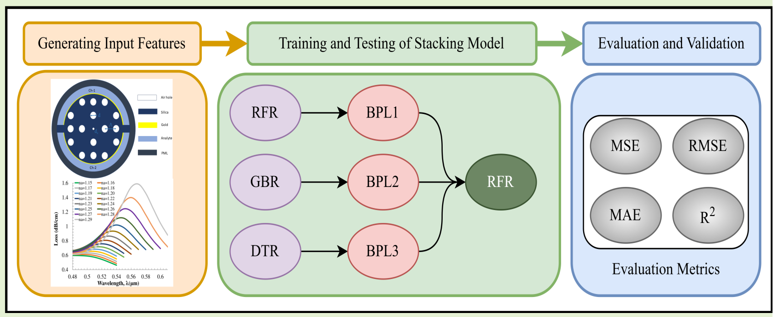
***Abstract*—In this paper, a photonic crystal fiber (PCF) surface plasmon resonance (SPR) sensor capable of detecting a wide range of refractive indices (RI) from 1.15 to 1.41 is designed and optimized using a stacking-based ensemble machine learning (ML) model. The stacking model is constructed using three regression models, including the random forest regressor (RFR), the gradient boosting regressor (GBR), and the decision tree regressor (DTR). To analyze the detection capabilities and different characteristics of the sensor, the finite element method (FEM)-based perfectly matched layer (PML) is applied as a boundary condition. A chemically stable noble plasmonic material, gold (AU), with a thickness of 40 nm, is used to create the SPR effect and placed on the outer layer of the fiber to make the sensor practically implementable. The numerical data from the FEM simulation were used to train and validate the proposed ML (ML) model. The proposed ML model provided an MSE value of 0.3584, an MAE of 0.2151, and a R^2 of 0.9769. In addition, various ablation studies were conducted to validate the proposed ML model and ensure its ability to design and optimize the multianalyte biosensor. The numerical findings demonstrate that the suggested sensor has a maximum amplitude sensitivity (AS) of -1204 RIU^{-1} and wavelength sensitivity (WS) of 10,000 nm/RIU. Due to its high sensitivity and simplified design, the presented sensor has the potential to be used to detect biochemical solutions, biological analytes, and gaseous molecules, with other lower RIs in the range of 0.5 to 2 μm, covering the visible to the near-infrared spectrum. The proposed ML model is highly capable and flexible for designing and optimizing multi-analyte biosensors, accordingly can be used for designing and optimizing other multi-analyte biosensors effectively.**



***Index Terms*—Simultaneous Detection; Sensitivity; Dual-analyte Sensor; Sensor Resolution; Machine Learning; Ensemble Model.**

I. Introduction

MANY research studies have been conducted on the PCF-based SPR sensing technology because of its compact size, ability to detect multiple analytes, and capability for remote sensing in different applications, including water and environmental quality monitoring, food safety, biochemical and gaseous molecule identification, and so on [1], [2]. Plasmons, which generate powerful local fields known as plasmonic surface waves (PSWs), guiding over the boundary in the form of traveling waves called surface plasmonic polaritons (SPPs), are the collective vibrations of charge at the boundary of a metal and a dielectric [3]. Through the connection of the electromagnetic field to highly energized particles found in plasmonic materials, including copper, aluminum, silver, and gold, SPPs can be developed between metal and dielectric interfaces, which results in a major portion of the optical energy being converted from the core to SPP mode, leading to a sharper resonance peak [4]. Selecting suitable plasmonic materials is crucial for designing a practical sensor. As a result of its sharpened resonance peak and not having an interband transition, silver is regarded as a superior plasmonic material. However, the material's excessive oxidation properties prevent its broad use in aqueous environments. On the other

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