Title: Simultaneous dual-analyte detection biosensor through a stacking-based ensemble machine learning approach: design and optimization

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Abastact: 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 is 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 model. The proposed ML model provided an MSE value of 0.3584, an MAE of 0.2151, and an R^2 of 0.9769. In addition, various 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, it can be used for designing and optimizing other multi-analyte biosensors effectively.

Keywords:

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