

Chapter

Recent Advances in Artificial Intelligence and Machine Learning Based Biosensing Technologies

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Abstract

Advancements in artificial intelligence (AI) and machine learning (ML) have transformed biosensing technologies, enhancing data acquisition, analysis, and interpretation in biomedical diagnostics. This chapter explores AI integration into biosensing, focusing on natural language processing (NLP), large language models (LLMs), data augmentation, and various learning paradigms. These technologies improve biosensor sensitivity, precision, and real-time adaptability. NLP automates biomedical text extraction, while LLMs facilitate complex decision-making using vast datasets. Data augmentation mitigates dataset limitations, strengthening ML model training and reducing overfitting. Supervised learning drives predictive models for disease detection, whereas unsupervised learning uncovers hidden biomarker patterns. Reinforcement learning optimizes sensor operations, calibration, and autonomous control in dynamic environments. The chapter discusses case studies, emerging trends, and challenges in AI-driven biosensing. AI's convergence with edge computing and Internet of Things (IoT)-enabled biosensors enhances real-time data processing, reducing latency and expanding accessibility in resource-limited settings. Ethical concerns, including data privacy, model interpretability, and regulatory compliance, must be addressed for responsible AI applications in biosensing. Future research should focus on developing AI models resilient to bias, capable of continuous learning, and optimized for low-power, portable biosensors. Addressing these challenges will enable AI-powered biosensing to advance precision medicine and improve global healthcare outcomes. Through interdisciplinary approaches, AI and ML will continue to drive the evolution of next-generation diagnostic solutions.

Keywords: artificial intelligence, biosensing, machine learning, large language models, natural language processing, blockchain

1. Introduction

Biosensors are analytical systems designed to detect specific molecules (analytes) by utilizing biorecognition elements that interact with the target and generate measurable signals [1]. These devices typically consist of four components: the analyte,

recognition element, transducer, and data handling mechanism (**Figure 1**) [2, 3]. Analytes can range from ions and small molecules to nucleic acids, proteins, viruses, or even cells, often serving as biomarkers for health, environmental monitoring, or drug discovery [4–6]. Recognition elements provide specificity and may include protein-based molecules like enzymes and antibodies, nucleic acid-based components such as Deoxyribonucleic Acid (DNA), Ribonucleic Acid (RNA), or aptamers, and artificial materials like molecularly imprinted polymers (MIPs) (**Figure 1**). The transducer converts the interaction between the analyte and recognition element into measurable signals using methods like electrochemical, colorimetric, optical, acoustic, or piezoelectric techniques [7, 8]. Data handling encompasses the acquisition, analysis, and interpretation of this information, with advanced biosensors integrating these processes into seamless, self-sufficient platforms (**Figure 1**). Effective biosensor development requires careful consideration of analyte relevance, recognition specificity, transduction sensitivity, and data interpretation to ensure precision and adaptability for diverse real-world applications. Biosensors come in a wide range of types including,

1. *Electrochemical biosensors*: These sensors detect changes in electrical properties, such as current, voltage, or impedance, caused by a biochemical reaction [9]. Common applications include glucose monitoring and environmental testing [10].

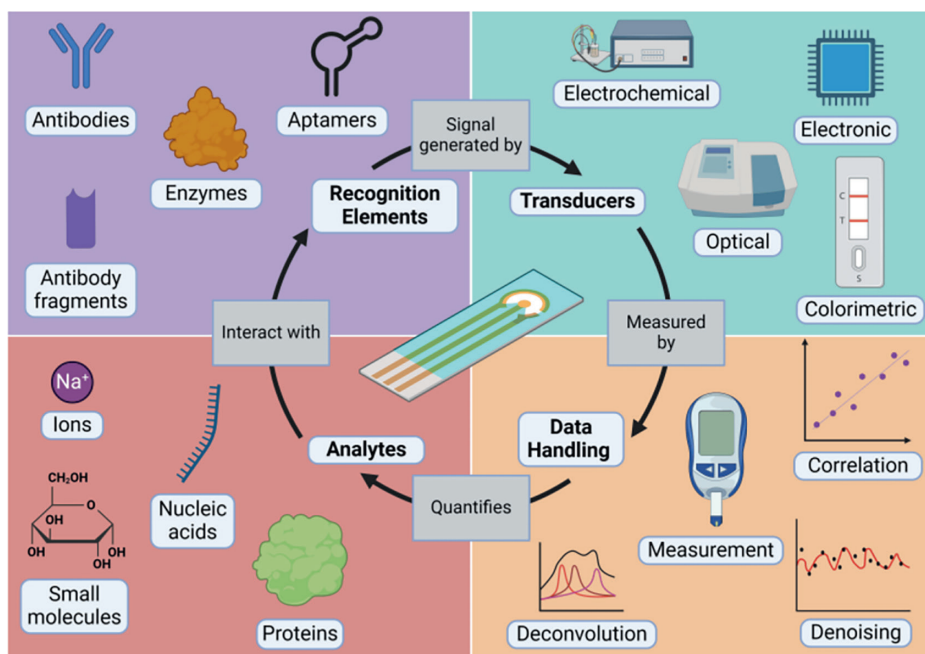


Figure 1. Schematic representation of the biosensor components and their functions. A biosensor consists of analytes (ions, proteins, nucleic acids, etc.) interacting with recognition elements (antibodies, enzymes, aptamers, etc.), which generate a signal. This signal is transduced via various mechanisms (electrochemical, optical, colorimetric, etc.) and processed through data handling systems for measurement, correlation, deconvolution, and denoising to quantify the analyte of interest. This was taken from Ref. [1].

2. *Optical biosensors*: These biosensors utilize light to analyze analyte interactions; optical sensors often leverage techniques such as fluorescence, surface plasmon resonance (SPR), and localized surface plasmon resonance (LSPR) [11, 12]. They are widely used in diagnostics and environmental monitoring. There has also been extensive work done that integrates quantum states of light with optical biosensors to increase the precision and signal-to-noise ratio (SNR) of the biosensors [13–23].
3. *Piezoelectric biosensors*: These sensors measure changes in mass or mechanical properties on a sensor surface due to molecular interactions [24–26]. Quartz crystal microbalances are a common example [27].
4. *Thermal biosensors*: These devices detect changes in temperature resulting from biochemical reactions, providing a measure of the analyte concentration [28].
5. *Magnetic biosensors*: These rely on the magnetic properties of labeled molecules to detect specific interactions [29]. They are often used in clinical diagnostics for detecting biomarkers.

Artificial intelligence (AI) refers to the simulation of human intelligence processes or processes that would otherwise require human intelligence by machines, particularly computer systems [30–33]. It encompasses a wide range of technologies and techniques that enable systems to perceive, reason, learn, and make decisions based on data inputs. AI systems are designed to perform tasks that typically require human intelligence, such as visual perception, natural language understanding, decision-making, and problem-solving. AI can be broadly categorized into:

- *Narrow AI*: Focused on performing specific tasks (e.g., voice assistants, recommendation systems) [34].
- *General AI*: Aims to replicate human-level intelligence across a wide range of activities (still largely theoretical) [34].

Machine learning (ML) is a subset of AI that focuses on enabling systems to learn and improve from experience without being explicitly programmed [35–38]. Machine learning algorithms analyze and process data to recognize patterns, make predictions, or generate insights in biosensing data [38–40]. The learning process involves using statistical models and computational techniques to “train” algorithms on datasets, enabling them to make decisions or predictions when exposed to new, unseen data. Machine learning algorithms can further be subdivided into:

- *Supervised learning*: Here algorithms learn from labeled datasets to predict outcomes (e.g., regression, classification) [41–44]. A subclass of supervised learning is semi-supervised learning, which is a type of machine learning paradigm that combines a small amount of labeled data with a large amount of unlabeled data during training. It lies between supervised learning, which uses fully labeled datasets, and unsupervised learning, which uses entirely unlabeled datasets [45].
- *Unsupervised learning*: Here the algorithms identify patterns and structures in unlabeled data (e.g., clustering, dimensionality reduction).

- **Reinforcement learning:** Here the algorithm learns to make decisions by interacting with an environment and maximizing rewards (e.g., game-playing algorithms, robotics) [46–50].

Together, AI and ML drive advancements across diverse fields, including healthcare, finance, transportation, and more, enabling intelligent automation and enhanced decision-making capabilities. Artificial intelligence has emerged as a transformative tool in biosensing, extending beyond data analysis to impact every stage of biosensor development, including analyte selection, recognition element discovery, signal transduction enhancement, and data handling. In analyte selection, AI-integrated omics approaches help identify biomolecular pathways and biomarkers, enabling the discovery of novel targets for complex diseases like cancer and Alzheimer's. Artificial intelligence aids biomarker discovery using machine learning algorithms for classification and clustering, facilitating multi-analyte analysis for comprehensive molecular profiling. This enhances diagnosis and treatment predictions by uncovering interconnected biomolecular signatures. Artificial intelligence and ML have transformed the landscape of biosensing, particularly in biomedical diagnostics, by enabling unprecedented capabilities in data acquisition, analysis, and interpretation. This chapter examines the integration of advanced AI methodologies, including NLP, LLMs, and various learning paradigms such as supervised, unsupervised, and reinforcement learning, into biosensing applications. By exploring these innovations, we aim to uncover how AI and ML elevate biosensor sensitivity, precision, and adaptability, driving real-time diagnostics to new heights.

2. AI-driven enhancements in biosensing sensitivity and precision

Artificial intelligence methodologies are instrumental in amplifying biosensor performance [51]. By leveraging machine learning models trained on vast datasets, biosensors can achieve highly refined detection and classification capabilities, crucial for identifying minute biomolecular changes that can be indicative of various diseases. In this section, we review the integration of AI techniques, such as feature extraction and pattern recognition, that significantly improve sensor sensitivity and data precision. For recognition element selection, AI accelerates the discovery of high specificity bioreceptors through top-down approaches like Systematic Evolution of Ligands by Exponential Enrichment (SELEX), optimized with tools such as AptaCluster and AlphaFold for structural predictions [1, 52]. AI also supports the bottom-up design of novel recognition elements, enabling the creation of *de novo* proteins, nucleic acids, and catalysts tailored for biosensing applications. In signal transduction, AI improves material design, miniaturizes instrumentation for point-of-care (POC) use, and enables biorecognition-free sensing by identifying patterns in nonspecific data, broadening the scope of biosensing technologies. Artificial intelligence's role in data handling includes optimizing data acquisition, reducing noise, and enhancing real-time performance through adaptive algorithms and dimensionality reduction techniques. In data analysis, machine learning models process complex datasets to classify, predict, and interpret biomolecular interactions with high accuracy. Finally, AI improves diagnostic precision by integrating heterogeneous data sources, supporting personalized healthcare and holistic patient management. Artificial intelligence can be applied to a wide range of areas in

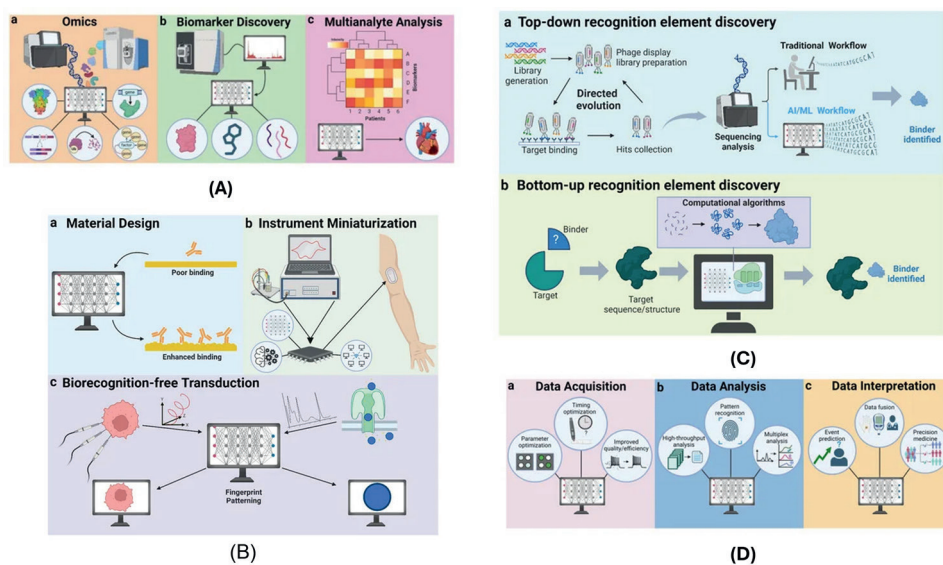


Figure 2. Schematic representation of the application of artificial intelligence approaches in biosensing to (A) analyte discovery and understanding, (B) biosensor transduction, (C) recognition element discovery, and (D) data handling [1].

biosensing, including analyte discovery and understanding, biosensor transduction, recognition element discovery, and data handling (Figure 2). Overall, AI follows a systematic workflow involving problem identification, data acquisition, model training, and application. By leveraging its pattern recognition capabilities, AI transforms biosensing into a more efficient, accurate, and scalable tool for healthcare and research.

The applications shown in Table 1 showcase AI's ability to enhance biosensor development and performance across multiple stages, from design and discovery to real-world deployment. Artificial intelligence in scientific research can be thought of as a tool that follows a standard workflow to address specific problems (Figure 3). The process begins with identifying a clear and actionable problem, such as the lack of a biorecognition element for a protein. Next, researchers gather relevant data, even if indirectly related, to inform their model. This data is then used to train the AI model, which identifies patterns and relationships to address the problem. The final step involves applying the model and optimizing it through validation and refinement to produce useful results. For example, AI can be used to predict or design a receptor for an unknown protein. By understanding this straightforward workflow, researchers can effectively integrate AI into their work.

3. The role of natural language processing (NLP) in biomedical knowledge synthesis

Natural language processing (NLP) has emerged as a powerful tool in biosensing, particularly for automating the extraction and synthesis of biomedical text data [53]. Natural language processing enables the development of knowledge bases from scientific literature, medical records, and diagnostic data, offering insights into

| Area | Applications |
|--------------------------------------|---|
| Analyte Selection | <ul style="list-style-type: none"> • Omics-based analysis to identify biomarkers and molecular pathways. • Discovery of novel biomarkers for diseases like cancer, Alzheimer's, and diabetes. • Multi-analyte analysis for molecular profiling and enhanced diagnostics. |
| Recognition Element Selection | <ul style="list-style-type: none"> • High-throughput screening of bioreceptors (e.g., aptamers, antibodies). • Top-down discovery using SELEX and machine learning algorithms. • Bottom-up design of <i>de novo</i> recognition elements, including proteins, nucleic acids, and enzymes. |
| Signal Transduction | <ul style="list-style-type: none"> • Design and optimization of metamaterials for improved optical and electrochemical sensors. • Miniaturization of biosensing instruments (e.g., spectrometers, potentiostats). • Biorecognition-free biosensors using pattern recognition in nonspecific data. |
| Data Handling | <ul style="list-style-type: none"> • Data acquisition: Real-time optimization of sensor parameters using reinforcement learning and adaptive algorithms. • Data analysis: Processing large datasets, pattern recognition, classification, and multiplexed sensing. • Data interpretation: Integration of time series data and heterogeneous data sources for personalized diagnostics. |
| Biosensor Development Workflow | <ul style="list-style-type: none"> • AI-assisted design and testing of biosensor components. • Workflow optimization to identify problems, train models, and validate designs. |
| Material and Instrument Design | <ul style="list-style-type: none"> • Development of new materials with tailored properties for sensing applications. • Intelligent design of miniaturized and wearable biosensors. |
| Diagnostics and Real-Time Monitoring | <ul style="list-style-type: none"> • Enhanced point-of-care (POC) diagnostics and wearable sensor technologies. • Prediction of disease progression and treatment responses using AI-based models. |

Designed using information from Ref. [1].

Table 1.

This table lists applications of artificial intelligence in biosensor development across different areas.

disease biomarkers, treatment guidelines, and emerging diagnostic methodologies. In this section, we discuss NLP applications that facilitate rapid updates to biosensor databases and the development of responsive, knowledge-driven diagnostic tools. Integrating NLP and large language models (LLMs) into biosensing technologies has significantly advanced biomedical diagnostics. NLP facilitates the analysis of unstructured data, such as patient records and sensor annotations, enabling the extraction of pertinent information and the identification of correlations between clinical findings and biosensor outputs. Large language models enhance this capability by interpreting multimodal data, including sensor readings and textual annotations, to provide comprehensive insights. This integration improves the sensitivity and precision of biosensors through adaptive learning from extensive datasets, leading to reduced false positives and negatives. Additionally, LLMs serve as AI assistants in biosensing

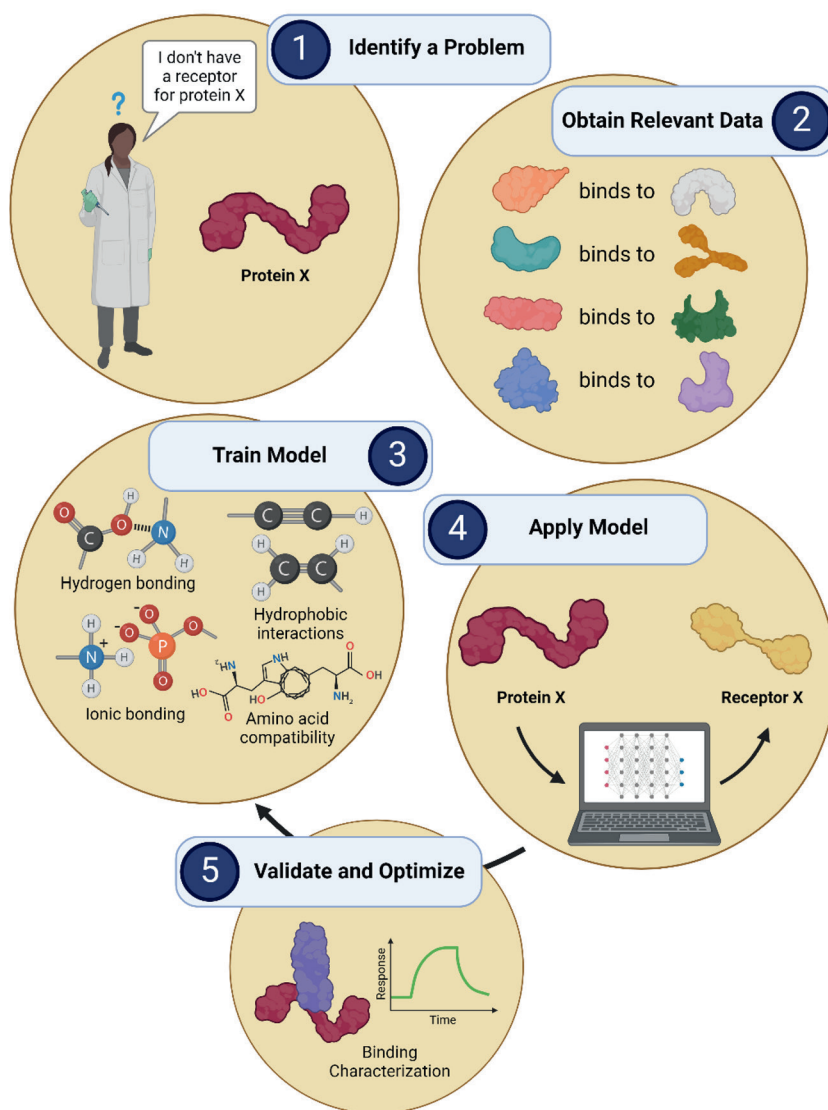


Figure 3. Schematic representation of the general workflow for artificial intelligence-assisted model development, illustrating the steps of (1) identifying a problem, (2) obtaining relevant data, (3) training the model, (4) applying the model, and (5) validating and optimizing the results for scientific applications. Taken from Ref. [1].

laboratories, offering real-time feedback, suggesting optimization strategies, and automating literature reviews to keep researchers informed of the latest advancements. However, challenges such as data privacy, the need for domain-specific training, and the necessity for interdisciplinary collaboration must be addressed to fully realize the potential of NLP and LLMs in biosensing. Studies like “Health-LLM: Large Language Models for Health Prediction via Wearable Sensor Data” and “LLMSense: Harnessing LLMs for High-level Reasoning Over Spatiotemporal Sensor Traces” [54, 55] exemplify the application of LLMs in processing and interpreting biosensor data, highlighting their role in advancing health prediction and high-level reasoning over sensor traces.

4. Large language models (LLMs) in decision-making and complex analysis

Large language models can be categorized into three main architectures: encoder-only, decoder-only, and encoder-decoder (**Figure 4**), each designed for specific tasks. Encoder-only models, like the Bidirectional Encoder Representations from Transformers (BERT), process input data to generate a fixed-size representation, making them suitable for tasks like classification and clustering [57–60]. These models are also applied in bioinformatics to learn representations of protein sequences. Decoder-only models, such as the Generative Pre-trained Transformer (GPT) series, focus on generating sequences or expanding information based on a seed input, making them ideal for tasks like text generation or sequence prediction in genomics. Encoder-decoder models, like T5 (Text-to-Text Transfer Transformer), specialize in sequence-to-sequence tasks, with the encoder creating a context-rich representation and the decoder generating an output sequence [61–63]. These are particularly useful for molecule captioning, editing, and summarization. Large language models are trained in two stages: pre-training and fine-tuning. Pre-training involves exposing the model to a vast corpus of scientific literature, enabling it to learn scientific terminology and concepts. The objective function varies by model architecture, with BERT using masked language modeling and GPT using autoregressive modeling. Fine-tuning adapts the pre-trained model to specific tasks by training it on labeled datasets. For example, chemical reaction classification uses annotated reaction samples, while generation tasks rely on input-output instruction pairs. The training pipeline for scientific LLMs, including textual, molecular, and genomic models, aligns closely with general LLM training workflows. LLMs are transforming decision-making in biosensing by analyzing and interpreting vast biomedical datasets to aid complex diagnostics. These models can enable biosensors to process intricate queries, recognize multifaceted disease markers, and support clinical decision-making processes.

Large language models are advanced deep learning models designed for NLP tasks such as machine translation, text summarization, paraphrasing, and text generation. Leveraging transformer architectures, LLMs capture long-range dependencies better than sequential models like Recurrent Neural Networks (RNNs). They can be fine-tuned for specific applications, making them versatile for niche tasks or as the backbone for general-purpose chatbots. OpenAI's GPT-3 has been widely used as the foundation for applications like JasperChat for business use and Poe by Quora. Beyond generic applications, LLMs have demonstrated potential in specialized domains such as healthcare.

The release of ChatGPT has highlighted LLMs' applicability in assisting healthcare practitioners. ChatGPT, pre-trained on vast textual data, can generate human-like responses and has even passed sections of the U.S. medical licensing exam, underscoring its proficiency with medical queries. For instance, Wang et al. introduced ChatCAD, a system integrating LLMs with computer-aided diagnosis (CAD) tools. ChatCAD converts outputs from image classifiers and segmentors into prompts for LLMs, leveraging their reasoning capabilities to improve patient care. ChatGPT's potential applications in healthcare include aiding clinical decision-making, assisting with patient interaction, and generating medical reports. Its ability to process and respond to medical queries positions it as a transformative tool in healthcare innovation.

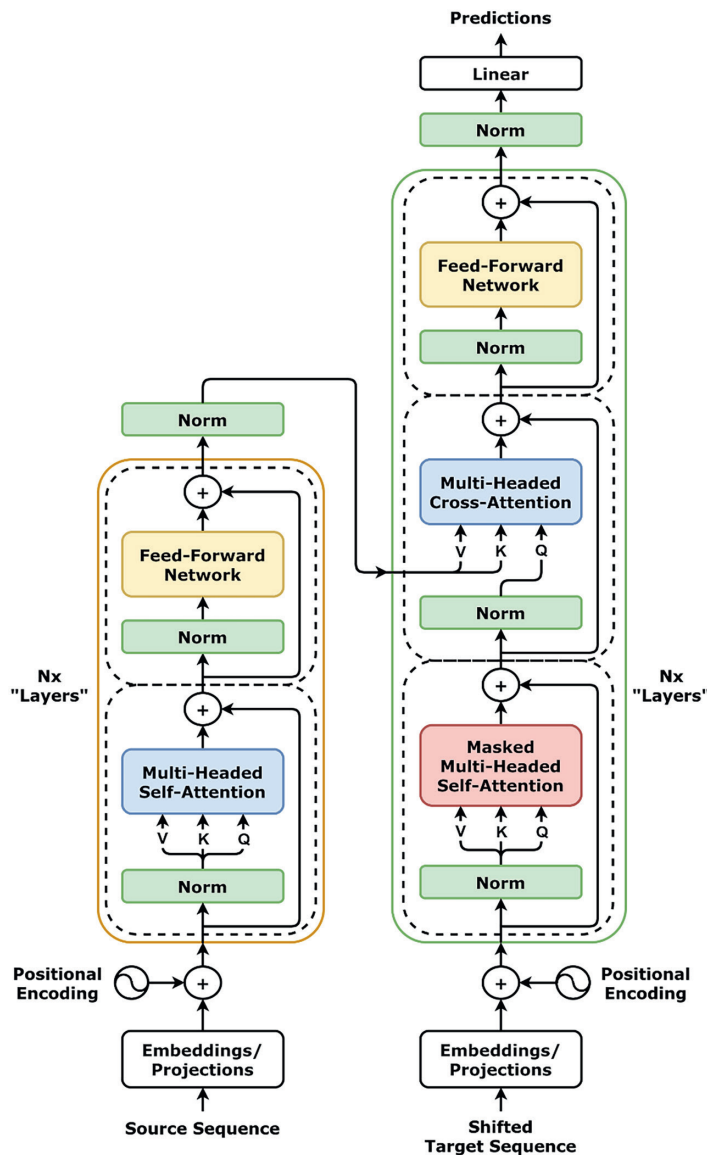


Figure 4. Illustration of the transformer architecture showcasing the encoder-decoder structure. The encoder processes input embeddings through layers of multi-head attention and feed-forward networks with residual connections and normalization. The decoder incorporates masked multi-head attention for sequential generation, enabling predictions for output probabilities through a linear layer followed by a softmax function. Taken from Refs. [56].

5. Data augmentation for overcoming biosensing dataset limitations

Data augmentation is a method used to increase the size and variability of datasets by creating modified versions of existing data [64–66]. It aims to address challenges such as overfitting, data scarcity, and high costs associated with collecting and labeling data. This section explores various augmentation techniques across different data types, including images, audio, text, and advanced applications, with an emphasis

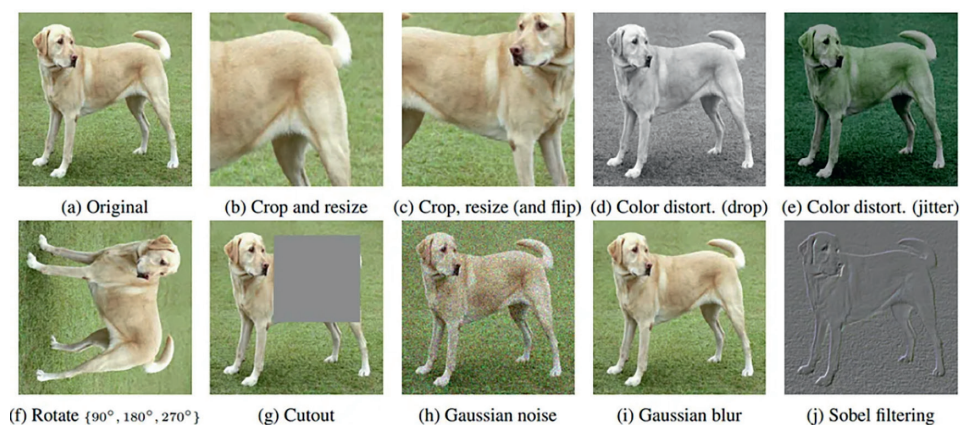


Figure 5. Example of data augmentation techniques used in SimCLR. These techniques, including cropping, resizing, flipping, color distortion (drop and jitter), rotation, cutout, Gaussian noise, Gaussian blur, and Sobel filtering, create multiple augmented “views” of the same sample. This process enhances model robustness by mapping different representations to a similar feature space. Taken from Ref. [67].

on tools such as Keras and TensorFlow. Data augmentation techniques are essential in biosensing due to the scarcity of high-quality, labeled datasets. We explore various augmentation strategies, including image transformations, synthetic data generation, and domain adaptation, that enhance model robustness. By creating more diverse training datasets, data augmentation helps reduce overfitting, enabling ML models to generalize more effectively and improve diagnostic accuracy across varied patient populations. Photometric data augmentation enhances model performance in projection radiography by applying techniques like cropping, flipping, color distortion, and noise addition to diversify the dataset (**Figure 5**) [67]. These augmentations improve the model’s robustness and ability to generalize by creating varied representations of the same input.

6. Heuristic, metaheuristic, and optimization for biosensing

A heuristic is a problem-solving approach that uses practical methods or rules of thumb to find a satisfactory solution efficiently, especially when exact methods are computationally expensive or infeasible [68]. In biosensing, heuristics can guide decision-making processes such as sensor design, parameter tuning, or signal analysis by providing approximate solutions based on domain knowledge. A meta-heuristic is a higher-level strategy designed to explore the solution space of complex optimization problems by combining and improving heuristic techniques. In biosensing, meta-heuristics like genetic algorithms, simulated annealing, or particle swarm optimization are employed to optimize sensor configurations, maximize sensitivity, or improve data analysis performance by balancing exploration and exploitation of the solution space. Optimization in biosensing refers to the process of finding the best parameters or configurations to achieve a desired objective, such as maximizing sensitivity, specificity, or detection speed, while minimizing cost or resource consumption. Optimization methods, including mathematical programming and machine learning, are used to enhance the performance of biosensing

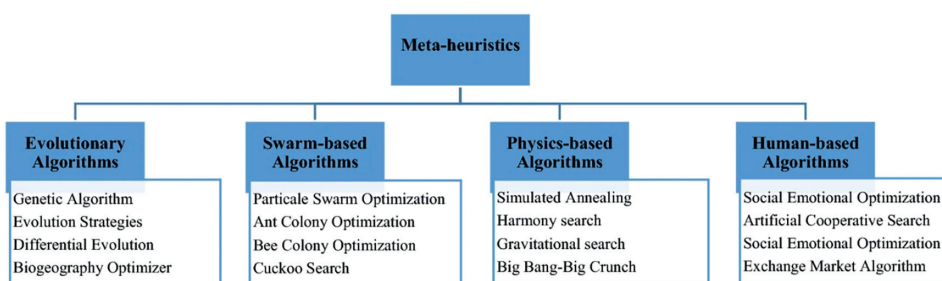


Figure 6. Classification of metaheuristic algorithms into four main categories—evolutionary algorithms, swarm-based algorithms, physics-based algorithms, and human-based algorithms—along with examples of each category, highlighting their diverse approaches to solving optimization problems [68].

systems, from material selection to device calibration and data interpretation. Metaheuristic algorithms (**Figure 6**) can significantly enhance biosensing by optimizing design, data analysis, and signal processing. Their applications are based on the four main categories:

6.1 Evolutionary algorithms

- Optimize biosensor design parameters (e.g., geometry, material composition).
- Tune operational parameters (e.g., temperature, pH) for improved detection.
- Select relevant features from high-dimensional datasets to enhance accuracy.

6.2 Swarm-based algorithms

- Optimize signal transduction mechanisms to improve sensitivity.
- Cluster biosensor data for categorizing analytes or patient samples.
- Configure multiplexed biosensors for simultaneous multi-analyte detection.

6.3 Physics-based algorithms

- Optimize material properties (e.g., surface composition) for enhanced transduction.
- Calibrate biosensors for accurate and reliable measurements.
- Reduce noise in biosensor signals for precise analyte quantification.

6.4 Human-based algorithms

- Aid in clinical decision-making by integrating biosensor outputs with patient data.
- Enable collaborative optimization for wearable and networked biosensors.

- Train AI-based biosensing platforms for interpreting complex data patterns.

These algorithms can improve biosensor sensitivity, specificity, cost-efficiency, and adaptability, facilitating advancements in healthcare, environmental monitoring, and food safety applications.

7. Supervised learning for predictive disease detection

Supervised learning is a branch of ML where a model is trained on a labeled dataset [42]. Each training example consists of input data (features) and the corresponding correct output (labels or targets). The algorithms (Table 2) learn to map inputs to outputs by minimizing the error between predicted and actual outcomes. Supervised learning is widely used in tasks like classification (categorizing data into predefined classes) and regression (predicting continuous values) [42]. Supervised learning is foundational in predictive modeling within biosensing. By training models on annotated data, supervised ML techniques allow ML-enhanced biosensors to recognize disease patterns and detect biomarkers with high specificity. This section covers the development of disease-specific models, feature selection methodologies, and the optimization of classification algorithms that contribute to early and accurate diagnosis.

| Algorithm | Type | Description |
|----------------------------------|-------------------------------|---|
| Linear Regression | Regression | Models the relationship between a dependent and one or more independent variables by fitting a linear equation. |
| Logistic Regression | Classification | Predicts probabilities and classifies data using a logistic (sigmoid) function. |
| Decision Tree | Classification/ Regression | Splits data into branches based on feature thresholds for prediction. |
| Random Forest | Classification/ Regression | Uses an ensemble of decision trees to improve prediction accuracy and reduce overfitting. |
| Support Vector Machine (SVM) | Classification/ Regression | Finds the hyperplane that best separates classes in the feature space. |
| K-Nearest Neighbors (KNN) | Classification/ Regression | Predicts the class or value of a data point based on the majority vote or average of its k-nearest neighbors. |
| Naïve Bayes | Classification | Applies Bayes' Theorem with the assumption of feature independence to classify data. |
| Gradient Boosting Machines (GBM) | Classification/ Regression | Builds models sequentially to minimize errors using gradient-based optimization. |
| XGBoost | Classification/ Regression | An optimized version of GBM with faster computation and additional features. |
| AdaBoost | Classification/ Regression | Combines weak classifiers to form a strong classifier by iteratively focusing on misclassified instances. |
| CatBoost | Classification/ Regression | A gradient boosting algorithm optimized for categorical features. |
| LightGBM | Classification/ Regression | A fast, distributed, high-performance GBM for large datasets. |

| Algorithm | Type | Description |
|-------------------------------------|-------------------------------|---|
| Neural Networks (MLP) | Classification/ Regression | Mimics the human brain to learn patterns in data through interconnected layers of neurons. |
| Convolutional Neural Networks (CNN) | Classification | Specializes in analyzing visual data by capturing spatial and temporal dependencies. |
| Recurrent Neural Networks (RNN) | Sequence Modeling | Models sequential data, such as time series, by utilizing feedback loops to process previous outputs. |
| Long Short-Term Memory (LSTM) | Sequence Modeling | A type of RNN designed to capture long-term dependencies in sequential data. |
| Transformers | Sequence Modeling | Leverages attention mechanisms for natural language processing and sequential data tasks. |
| Ridge Regression | Regression | A linear regression model with L2 regularization to prevent overfitting. |
| Lasso Regression | Regression | A linear regression model with L1 regularization to enforce sparsity in feature selection. |

Table 2.
 This table shows a list and descriptions of supervised learning algorithms, covering classical and deep learning approaches.

8. Unsupervised learning for biomarker discovery and pattern recognition

Machine learning that operates without labeled data is called unsupervised learning [69]. This approach involves algorithms designed to identify patterns, structures, or relationships within unlabeled datasets. The primary objective is to extract meaningful insights, such as grouping similar data points into clusters or uncovering hidden structures within the data. Unsupervised learning has diverse applications, including feature reduction, anomaly detection, and data visualization [70]. One prominent use of unsupervised learning is in clustering, where data is organized into groups based on similarities. Clustering algorithms, such as K-means, Hierarchical Clustering (HC), Density-Based Spatial Clustering of Applications with Noise (DBSCAN), and Spectral Clustering (SC), aim to partition data into clusters of similar objects. These techniques are widely applied in tasks like customer segmentation, market analysis, and image segmentation. In the context of healthcare, clustering can be used to identify patient subgroups with distinct biomarker profiles, offering insights into different disease outcomes or treatment responses. Another critical application of unsupervised learning is dimensionality reduction, where the goal is to reduce the number of features in a dataset while retaining essential information. Techniques like Principal Component Analysis (PCA) are commonly employed to simplify data, improve computational efficiency, and minimize overfitting. This is especially valuable in fields like biomarker discovery, where researchers can focus on the most relevant biomarkers for a specific condition, enhancing the robustness and interpretability of the analysis.

Association rule learning is another unsupervised approach that identifies correlations and frequent item combinations within large datasets [71]. In biomarker research, association rule mining can reveal sets of biomarkers with co-expression or co-regulation patterns, suggesting their involvement in shared biological pathways or processes. This technique complements other unsupervised methods by uncovering complex interrelationships in high-dimensional data. **Table 3** provides a

comprehensive overview of various classical and deep learning based unsupervised learning algorithms. It includes clustering methods, dimensionality reduction techniques, and advanced neural network-based approaches. These algorithms are widely used in tasks such as grouping data points, reducing feature dimensionality, detecting anomalies, and generating synthetic data. The table categorizes algorithms by type and highlights their key functionalities, offering a quick reference for selecting appropriate methods for unsupervised learning tasks.

Unsupervised learning, through clustering, dimensionality reduction, and association rule mining, offers powerful tools to explore and analyze unlabeled data, enabling breakthroughs in areas ranging from biomarker discovery to market segmentation and beyond. Unsupervised learning approaches are particularly valuable in identifying unknown biomarker patterns and latent structures within biosensing data. By clustering similar data points and detecting anomalies, these models facilitate biomarker discovery, a critical step in developing new diagnostic tools. Algorithms,

| Algorithm | Type | Description |
|--|--------------------------|---|
| K-Means | Clustering | Partitions data into k clusters based on minimizing variance within clusters. |
| Hierarchical Clustering | Clustering | Creates a tree of clusters using agglomerative (bottom-up) or divisive (top-down) approaches. |
| DBSCAN | Clustering | Groups points based on density, identifying clusters of varying shapes and sizes, and marking outliers. |
| Mean-Shift | Clustering | Locates regions of high data density and forms clusters around those regions. |
| Gaussian Mixture Models (GMM) | Clustering | Models the dataset as a mixture of multiple Gaussian distributions for soft clustering. |
| Spectral Clustering | Clustering | Uses graph theory and eigenvalues to cluster data points, especially for nonlinear relationships. |
| Affinity Propagation | Clustering | Identifies exemplars (cluster centers) using similarity measures rather than predefining the number of clusters. |
| Fuzzy C-Means | Clustering | Allows data points to belong to multiple clusters with varying degrees of membership. |
| Principal Component Analysis (PCA) | Dimensionality Reduction | Reduces dataset dimensionality by projecting it onto principal components that capture maximum variance. |
| Kernel PCA | Dimensionality Reduction | Extends PCA to nonlinear relationships using kernel functions. |
| t-SNE | Visualization | Maps high-dimensional data into two or three dimensions for visualization, preserving local relationships. |
| UMAP (Uniform Manifold Approximation and Projection) | Visualization | Similar to t-SNE but faster, preserving both local and global data structure. |
| Autoencoders | Deep Learning | Neural networks that encode data into a compressed representation and decode it back, useful for feature extraction and dimensionality reduction. |
| Variational Autoencoders (VAE) | Deep Learning | A probabilistic extension of autoencoders, generating new data similar to the input. |

| Algorithm | Type | Description |
|---|--------------------------|--|
| Generative Adversarial Networks (GANs) | Deep Learning | Two neural networks (generator and discriminator) compete to produce realistic synthetic data. |
| Restricted Boltzmann Machines (RBM) | Deep Learning | Energy-based models that learn a probabilistic representation of the data. |
| Self-Organizing Maps (SOM) | Clustering | Projects high-dimensional data onto a lower-dimensional grid, preserving the topological relationships. |
| Deep Belief Networks (DBN) | Deep Learning | Stack of RBMs trained layer-wise, often used for unsupervised pre-training in deep learning. |
| Non-Negative Matrix Factorization (NMF) | Dimensionality Reduction | Factorizes data into non-negative components, useful for parts-based representations (e.g., topic modeling). |
| Independent Component Analysis (ICA) | Dimensionality Reduction | Separates mixed signals into statistically independent components (e.g., separating audio sources). |
| Deep Clustering | Deep Learning | Combines clustering with deep feature extraction, using deep neural networks to improve clustering performance. |
| Self-Supervised Learning (SimCLR, BYOL, etc.) | Deep Learning | Learns representations by creating auxiliary tasks without labels, such as predicting transformations of input data. |
| Anomaly Detection with Isolation Forest | Anomaly Detection | Identifies outliers by isolating them through random partitioning of data. |
| Deep InfoMax (DIM) | Deep Learning | Maximizes mutual information between input data and its representations to learn meaningful features. |

Table 3.
 This table shows a list and descriptions of unsupervised learning algorithms, covering classical and deep learning approaches.

such as K-means clustering and principal component analysis (PCA), have yielded insights into complex biosensing datasets.

9. Reinforcement learning for sensor optimization and autonomous control

Reinforcement learning is a machine learning paradigm where an agent interacts with an environment to learn a policy that maximizes cumulative rewards over time [72, 73]. Reinforcement learning, much like the supervised and unsupervised learning classes, has a wide range of algorithms (Table 4). The agent takes actions based on its current state, receives feedback in the form of rewards, and updates its strategy to improve future performance. Reinforcement learning methods are broadly categorized into policy-based and value-based approaches. Policy-based algorithms, like REINFORCE and Actor-Critic, directly optimize the policy, making them suitable for continuous or stochastic action spaces, though they may converge slowly. Value-based methods, such as Q-Learning and Deep Q-Networks (DQN), estimate value functions to derive policies, excelling in discrete action spaces but struggling in continuous ones. Hybrid methods like Actor-Critic combine the strengths of both to balance sample efficiency and convergence. RL has applications in gaming, robotics, autonomous vehicles, and more. Reinforcement learning offers innovative solutions for optimizing biosensor operations in real-time, particularly in environments requiring adaptive

| Algorithm | Type | Description |
|--|--------------------|--|
| Q-Learning | Model-Free | Learns an action-value function (Q-table) that predicts the total expected reward for taking an action in a given state. |
| SARSA (State- Action- Reward-State-Action) | Model-Free | Similar to Q-Learning but updates the Q-value-based on the action actually taken by the policy. |
| Deep Q-Network (DQN) | Model-Free | Extends Q-Learning by using a neural network to approximate the Q-function for high-dimensional state spaces. |
| Double Q-Learning | Model-Free | Addresses the overestimation problem in Q-Learning by maintaining two Q-value estimates and updating them alternately. |
| Policy Gradient Methods | Policy-Based | Directly optimize the policy by maximizing the expected reward using gradient ascent methods. |
| Deep Deterministic Policy Gradient (DDPG) | Policy-Based | Combines policy gradients and actor-critic methods for continuous action spaces, using deep neural networks. |
| Trust Region Policy Optimization (TRPO) | Policy-Based | Optimizes policies while ensuring updates do not deviate far from the current policy to maintain stability. |
| Proximal Policy Optimization (PPO) | Policy-Based | A simpler, efficient alternative to TRPO that uses clipped surrogate objectives to constrain policy updates. |
| Actor-Critic Methods | Hybrid | Combines value-based and policy-based methods by having an actor learn the policy and a critic evaluate it. |
| Advantage Actor-Critic (A2C) | Hybrid | Improves actor-critic by using the advantage function to reduce variance in policy updates. |
| Asynchronous Advantage Actor-Critic (A3C) | Hybrid | Parallelizes training by running multiple agents simultaneously to speed up convergence. |
| Soft Actor-Critic (SAC) | Hybrid | Incorporates entropy maximization to encourage exploration, balancing exploration and exploitation effectively. |
| Monte Carlo Methods | Model-Free | Estimate the value function and policy by sampling complete episodes and using returns to update estimates. |
| Temporal Difference (TD) Learning | Model-Free | Combines ideas from Monte Carlo and Dynamic Programming by updating estimates based on partial episodes. |
| TD(λ) | Model-Free | A generalization of TD learning that combines one-step and multi-step predictions using a decay factor . |
| Hierarchical Reinforcement Learning | Hierarchical | Decomposes the task into a hierarchy of subtasks, allowing agents to learn at multiple levels of abstraction. |
| Evolution Strategies (ES) | Optimization-Based | Uses population-based optimization techniques to optimize policies without relying on gradients. |
| Bayesian Reinforcement Learning | Model-Based | Integrates uncertainty into model-based RL by using Bayesian approaches to handle incomplete knowledge. |
| Model-Based RL | Model-Based | Learns a model of the environment's dynamics to predict future states and optimize the policy accordingly. |
| Inverse Reinforcement Learning (IRL) | Inference-Based | Infers the reward function based on observing expert behavior to replicate it. |

Table 4. This table shows a list and descriptions of reinforcement learning algorithms, covering classical and deep learning approaches.

calibration and autonomous decision-making. By setting reward functions and enabling trial-and-error learning, reinforcement learning allows sensors to dynamically adjust to changing conditions, enhancing diagnostic reliability. This section highlights case studies demonstrating reinforcement learning's role in calibrating biosensors and automating routine tasks, including anomaly detection and response to environmental changes.

10. Blockchain technology in biosensing

Blockchain technology is emerging as a transformative tool in biosensing by enhancing data security, traceability, and trust in biosensor networks [74, 75]. Biosensors, particularly in healthcare, environmental monitoring, and food safety, generate vast amounts of sensitive and real-time data. Integrating blockchain with biosensing systems ensures that this data is tamper-proof, transparent, and decentralized, addressing key challenges such as data integrity, privacy, and trust. Blockchain offers secure, decentralized storage for biosensor data, ensuring that the data collected remains unaltered and protected from unauthorized access. In healthcare, patient biosensor data can be encrypted and recorded on a blockchain ledger, allowing only authorized stakeholders (e.g., doctors, researchers) to access it. This prevents breaches and aligns with privacy regulations like General Data Protection Regulation (GDPR) and Health Insurance Portability and Accountability Act (HIPAA). The immutable nature of blockchain enables end-to-end traceability of biosensor data. Each data point from biosensors can be timestamped and linked to its source, ensuring accountability. For example, in environmental monitoring, blockchain can trace pollutant data back to its origin, enhancing transparency in regulatory compliance. Blockchain supports distributed biosensing networks, where multiple biosensors share and validate data in a peer-to-peer system. This is particularly beneficial for IoT-based biosensors in smart healthcare or smart agriculture, where decentralized storage and consensus mechanisms prevent single points of failure and ensure reliability. Blockchain-based smart contracts automate data validation and management processes. For example, in food safety, a smart contract could trigger an alert when biosensors detect contaminants exceeding a threshold, ensuring rapid response.

Despite its potential, blockchain integration in biosensing faces challenges such as scalability, energy consumption, and the need for real-time processing capabilities. The computational requirements of blockchain can be a bottleneck, especially for biosensors generating large volumes of data. Future solutions, such as lightweight blockchain protocols and integration with edge computing, will help overcome these barriers. As blockchain technology continues to evolve, it is poised to revolutionize biosensors by ensuring secure, transparent, and reliable data management, particularly in healthcare, environmental monitoring, and supply chain applications.

11. Emerging trends and challenges in AI-enhanced biosensing

AI-enhanced biosensing is driving advancements in biomedical diagnostics, environmental monitoring, and personalized medicine by improving sensitivity, accuracy, and real-time analysis. Machine learning models, including supervised, unsupervised,

and reinforcement learning, are being applied to interpret complex biosensor data, detect patterns, and optimize performance. AI-driven signal processing enhances weak signals in optical and electrochemical biosensors, while smart wearable devices and microfluidic systems enable real-time health monitoring and lab-on-a-chip diagnostics. Multimodal biosensing platforms, which combine data from various sensors, further enhance detection capabilities. Emerging trends also include edge computing for low-latency wearable devices, explainable AI for clinical trust, and the integration of AI with quantum and nanobiosensing technologies for ultra-sensitive detection.

Despite its potential, AI-enhanced biosensors face several challenges. High-dimensional and complex biosensor datasets require significant computational resources for real-time processing, while limited labeled data can lead to poor model generalization. Embedding AI algorithms into portable or wearable biosensors remains constrained by hardware power and efficiency. Black-box AI models lack interpretability, creating barriers to clinical and regulatory adoption. Data security and privacy, especially for sensitive health information, present further obstacles, necessitating compliance with regulations like GDPR and HIPAA. Additionally, high implementation costs limit accessibility in low-resource settings, requiring innovations such as open-source AI tools and affordable biosensor platforms to drive broader adoption.

We analyze recent developments, such as the integration of biosensors with wearable technologies, multimodal AI models combining imaging and genetic data, and edge computing for localized data processing. This section also addresses challenges, including ethical considerations, data privacy, and model interpretability, that must be managed to achieve widespread adoption in clinical settings.

12. Conclusion and future directions and interdisciplinary approaches

The integration of AI and ML into biosensing technologies has significantly enhanced the sensitivity, precision, and real-time adaptability of biosensors. By leveraging AI methodologies such as supervised, unsupervised, and reinforcement learning, as well as tools like NLP and LLMs, biosensors can efficiently process complex datasets, improve signal detection, and uncover hidden patterns critical for biomarker discovery. Innovations in AI-driven signal processing, edge computing, and wearable biosensors have paved the way for advanced diagnostics, personalized healthcare, and environmental monitoring solutions. Furthermore, emerging technologies like blockchain are improving data security, traceability, and transparency, strengthening the reliability and trustworthiness of biosensing systems.

Despite these advancements, challenges remain in achieving seamless integration of AI into biosensing platforms. Issues such as high computational demands, limited labeled datasets, and hardware constraints hinder scalability and real-time performance, particularly in resource-limited settings. Black-box models and data privacy concerns further complicate clinical and regulatory adoption, emphasizing the need for explainable AI, lightweight models, and interdisciplinary collaboration. Moving forward, addressing these challenges through innovative solutions, open-source frameworks, and collaborative research will be essential in realizing the full potential of AI-enhanced biosensing. By overcoming these barriers, AI-driven biosensors are set to revolutionize diagnostics, enabling faster, more accurate, and cost-effective solutions across healthcare, industry, and environmental sectors.

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Conflict of interest

The authors declare no conflict of interest.

Nomenclature

| | |
|-------|---|
| AI | artificial intelligence |
| CAD | computer-aided diagnosis |
| DNA | deoxyribonucleic acid |
| RNA | ribonucleic acid |
| GAN | generative adversarial network |
| HIPAA | health insurance portability and accountability act |
| IoT | internet of things |
| LLM | large language model |
| MIP | molecularly imprinted polymers |
| LSPR | localized surface plasmon resonance |
| MEG | magnetoencephalography |
| ML | machine learning |
| MRI | magnetic resonance imaging |
| NLP | natural language processing |
| PCA | principal component analysis |
| POC | point-of-care |
| RL | reinforcement learning |
| SERS | surface-enhanced Raman spectroscopy |
| SNR | signal-to-noise ratio |
| SPR | surface plasmon resonance |
| SQUID | superconducting quantum interference device |
| TPU | tensor processing unit |
| SELEX | systematic evolution of ligands by EXponential enrichment |
| CNN: | convolutional neural network |
| DNN | deep neural network |
| DQN | deep Q-network |
| GAN | generative adversarial network |
| GBM | gradient boosting machine |
| KNN | K-nearest neighbors |
| LLM | large language model |
| LSTM | long short-term memory |
| ML | machine learning |
| NLP | natural language processing |
| NN | neural network |

| | |
|---------|---|
| NMF | non-negative matrix factorization |
| PCA | principal component analysis |
| RNN | recurrent neural network |
| RL | reinforcement learning |
| SVM | support vector machine |
| TRPO | trust region policy optimization |
| PPO | proximal policy optimization |
| UMAP | uniform manifold approximation and projection |
| VAE | variational autoencoder |
| XGBoost | extreme gradient boosting |

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