

# Deep Learning for Human Disease Detection, Subtype Classification, and Treatment Response Prediction through Epigenomic Data Analysis

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**Abstract:** A potent machine learning method that has shown impressive results in a variety of fields is deep learning (DL). Although its application to epigenomics for human disease prediction has been relatively unexplored until recently, it holds great potential to assist physicians and scientists. In this article, we present a critical review of published studies that employ DL models to predict disease diagnosis, subtype classification, and treatment outcomes using epigenomic data. 22 pertinent articles were included from an original pool of 1140 publications after a thorough search throughout PubMed, Scopus, Web of Science, Google Scholar, and arXiv.org in accordance with the Preferred Reporting Items for Systematic Reviews and Meta-Analyses standards. DNA methylation and RNA-sequencing data were the most frequently employed data types for training predictive models. Notably, the evaluated models' accuracies ranged from 88.3% to 100.0% for disease detection tasks, from 69.5% to 97.8% for subtype categorization tasks, and from 80.0% to 93.0% for treatment response prediction tasks. We propose a comprehensive workflow encompassing all stages of developing a predictive model, from defining human disease-related tasks to evaluating model performance. The integration of DL into epigenomic research shows promise for transforming big data into valuable knowledge, thereby advancing translational epigenomics.

**Keywords:** deep learning; epigenomics; disease detection; subtype classification; treatment response prediction; systematic review.

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## 1. Introduction

Deep learning (DL) has emerged as a powerful neural-network-based method with multiple hidden layers, making it a leading paradigm in machine learning (ML) for classification and regression tasks [1,2]. Its success lies in its ability to handle extensive, high-dimensional, and complex structured data across various fields of study [3]. Over the last

decade, DL has played a vital role in bioinformatics and systems biology, enabling valuable insights from the exponentially increasing volume of omics data [4].

Epigenetics, introduced by Conrad Waddington in 1942, encompasses the study of heritable changes in gene function that do not involve alterations in DNA sequence, making it a promising approach for managing complex diseases [5]. The epigenomic status of cells and tissues is influenced by various events, including DNA and histone modifications, which can be affected by environmental factors [6]. By constructing a comprehensive genome-wide catalog of epigenetic control elements and understanding their changes in different cell states, crucial insights into the connections between environmental exposure, genotype, and phenotype can be gained [7]. The presence of epigenetic biomarkers has been extensively studied across a wide range of human diseases, offering potential benefits for early detection, subtype classification, prognosis, and prediction of response to therapy [8-10]. As a result, translational epigenomics, aiming to leverage associations between epigenomic marks and clinical outcomes, has garnered significant attention in recent years [11].

The rapid advancement of epigenomics has posed significant challenges for traditional analysis methods in human disease-related classification and regression tasks, primarily due to the vast volumes of high-dimensional, high-throughput data involved. To address this issue, deep learning (DL) has emerged as a promising approach, leveraging epigenomic data to help medical professionals and researchers gain a deeper understanding of human diseases. While several review papers have been published on DL and epigenomics, only a limited number have explored their applicability to clinical practice. Literature reveals that improved interpretability of DL in epigenomics by demystifying its black-box nature [12,13]. However, most of these works have primarily focused on biological mechanisms and model structures rather than exploring the clinical outcomes of human diseases.

Similarly, previous reviews on cancer and rare diseases have highlighted the promising ability of DL to reveal the role of epigenomics in the pathophysiology of human diseases, offering new diagnostic tools and therapeutic opportunities. Numerous studies have emphasized the potential therapeutic uses of machine learning (ML) and epigenetics; nevertheless, their purview was limited, with the latter providing merely a list of illnesses or medical disorders without a thorough explanation, and the former focusing only on DNA methylation data. As we have witnessed rapid acceleration in the development of both deep learning (DL) and epigenomics over the last decade, it is foreseeable that their integration will play a crucial role in assisting physicians in clinical practice in the near future. However, the delay in this trend may be attributed to a lack of communication between researchers in the two domains. Epigenomics researchers, while possessing vast amounts of data, may be more familiar with conventional statistical methods and may not be well-versed in using DL techniques to fully leverage their data's potential. On the other hand, DL researchers may not have a strong understanding of epigenomic data and its unique characteristics.

This review seeks to bridge this gap and foster fruitful collaborations between researchers in DL and epigenomics. By providing a comprehensive review of DL-based predictive models in epigenomics for disease detection, subtype classification, and treatment response prediction, the paper aims to highlight the potential benefits of integrating these approaches.

Furthermore, the review will delve into the main characteristics of common epigenomic data types and potential data sources, particularly focusing on several publicly available databases that could serve as valuable resources for developing predictive models.

To enable successful integration, the review will also discuss data preprocessing flows, DL architectures, DL libraries, and model evaluation metrics well-suited to epigenomic data.

By addressing practical challenges and identifying future trends in the development of DL techniques for epigenomic data in translational medicine, the review will pave the way for the advancement of this interdisciplinary field.

## 2. Materials and Methods

We conducted this review following the Preferred Reporting Items for Systematic Reviews and Meta-Analyses (PRISMA) guidelines.

### 2.1. Search strategy.

A comprehensive search strategy was developed to identify relevant articles published through September 2023 across three major databases: PubMed, Web of Science, and Scopus. There were no restrictions on the data used in the search. The search queries were carefully constructed, combining keywords related to deep learning (DL) and various common neural network architectures, such as multi-layer perceptron, convolutional neural network, recurrent neural network, and autoencoder. Additionally, keywords related to epigenomic data, such as DNA methylation, histone modifications, and non-coding RNAs, were included. To ensure the thoroughness of the search, other sources were also utilized. A manual search was conducted on Google Scholar and arXiv.org to identify any additional relevant studies. Moreover, the bibliographies of the selected studies and key review papers were examined to identify potential articles that may have been missed in the initial database searches.

### 2.2. Study selection and eligibility criteria.

After importing initially identified articles to EndNote X9, we removed duplicates and then screened titles, abstracts, and full texts based on eligibility criteria as follows:

DL models or predictive models that utilize DL as a component to solve human disease-related tasks;

By excluding articles that did not directly pertain to clinical outcomes, our review focused on research with practical implications for medical professionals and researchers in translational medicine. This selection criterion ensures that the identified studies are relevant to the application of deep learning in epigenomics to improve disease diagnosis, classification, prognostication, and treatment selection, ultimately contributing to the integration of DL into clinical practice.

By limiting the scope to epigenomics, we aimed to provide a more coherent and in-depth review of how deep learning techniques are being applied to predict clinical outcomes from epigenomic data.

Only original works were included. Reviews, commentaries, and editorials were excluded.

Publications with unavailable full texts were discarded.

For works that were improved and published more than once, we selected the latest publication only. Any disagreements among the authors were resolved through discussion until a consensus was reached.

2.3. Data extraction.

We qualitatively synthesized the following data, synthesizing this information from the included studies. Our review aimed to provide a comprehensive overview of the application of deep learning in epigenomics for human disease-related prediction tasks. This synthesis allows us to identify common trends, patterns, and successful approaches that have been employed in this burgeoning field of research.

3. Results and Discussion

3.1. Selection results.

The study selection process involved identifying relevant articles from the initial pool of 1806 studies. After removing duplicates, the titles and abstracts of each remaining article were screened to determine eligibility. A total of 1016 articles were excluded at this stage. The full texts of the remaining 124 articles were then obtained and further screened to assess their suitability for inclusion in the review. Ultimately, 22 studies met the criteria and were included in the qualitative synthesis for the review.

3.2. An overview of DL in translational epigenomics.

The application of deep learning (DL) to assist physicians and scientists in clinical settings using epigenomic data has been relatively unexplored until recently. Of the 22 papers reviewed, only one was published before 2016, indicating that this is a novel, rapidly growing field of study. The majority of the reviewed papers were published within the last 5 years, with a significant number of research teams from the USA and China contributing to this emerging area. This trend suggests an increasing interest in the potential of DL in translational epigenomics.

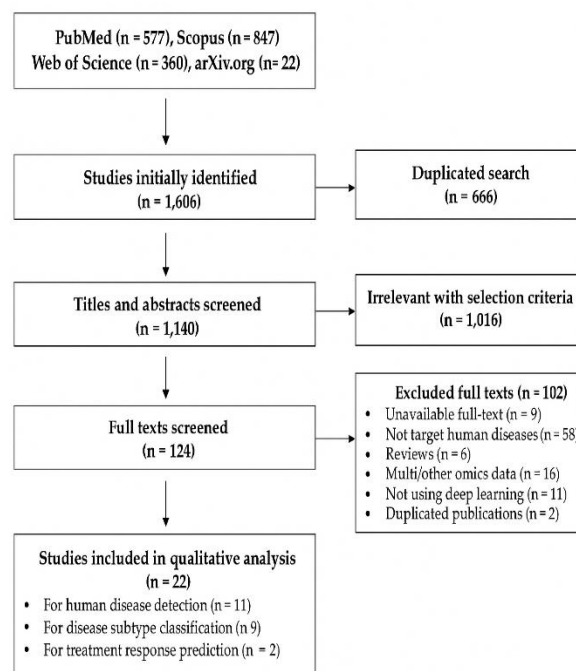


Figure 1. Workflow of DL models in tackling epigenomic data.

Within the domain of human disease-related tasks, disease detection, subtype classification, and treatment response prediction have received significant attention. Existing evidence indicates that DL models in epigenomics have demonstrated superior or at least competitive performance compared to traditional machine learning (ML) models. Notably, DL was used as a potent part of a multi-step procedure in several predictive models in earlier research. Regarding the types of epigenomic data used in these studies, DNA methylation and RNA sequencing (RNA-seq) were the most frequently employed, as shown in Figure 1. Various network architectures were utilized, including multi-layer perceptron, autoencoder and its variants, convolutional neural network, and deep belief network, highlighting the versatility of DL models in tackling epigenomic data.

A recent study was conducted using four deep neural networks (DNNs), including a multi-layer perceptron (MLP), long short-term memory (LSTM), convolutional neural network (CNN), and denoising autoencoder (DAE), to explore the capability of long non-coding RNA (lncRNA) in classifying eight different cancer types. CNN achieved the highest performance, while MLP had the poorest performance. The overall good classification results across all models suggest that lncRNA expression can be a significant feature for differentiating between multiple cancer types [14].

The Deep2Met model used preprocessed DNA methylation beta-values as input to a five-layer CNN to predict whether patients with colorectal cancer metastasized. The model achieved an impressive area under the precision-recall curve (AUPR) of 96.99%, which is critical for estimating performance with imbalanced class data. It also demonstrated high values of sensitivity, specificity, accuracy, precision, and F-score, indicating promise for diagnosing colorectal cancer based on individual patients' methylation profiles.

A class-incremental learning approach called Deep Generative Feature Reply was proposed for cancer classification tasks, showing superior accuracy. The model consists of an incremental feature selection process to identify the most significant CpG sites, and a scholar network that includes a variational autoencoder (VAE) as a generator to produce pseudo data without accessing past samples, and a neural network classifier to predict cancer types [15,16].

### *3.3. An Insight into epigenomic data used to train predictive models for human diseases.*

DNA methylation is one of the most extensively investigated epigenetic mechanisms due to its crucial role in gene expression regulation, including X-chromosome inactivation and the allele-specific silencing of imprinted genes, which are preferentially expressed from only one of the parental copies. The integration of traditional biochemical methodologies with novel bioinformatic analysis methods, such as deep learning (DL), has significantly advanced our understanding of DNA methylation patterns in various human diseases, including cancer, concussion, schizophrenia, and cardiovascular diseases.

Genome-wide profiling of DNA methylation can be performed using various sequencing technologies. Currently, DNA methylation levels are commonly represented as beta-values, which are the ratios of methylation intensity to the combined intensities of methylation and unmethylation at a particular CpG locus [17]. The beta-value of each CpG locus is calculated using the following formula.

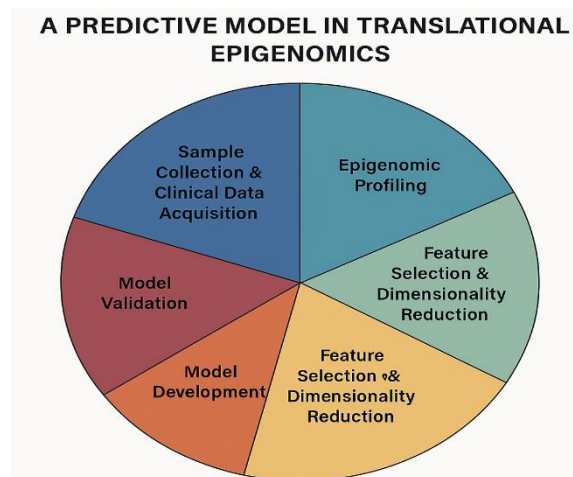
$$\beta = \text{Max}(I_M, 0) / \{\text{Max}(I_M, 0) + \text{Max}(I_U, 0) + \alpha\} \quad (1)$$

The combination of traditional experimental approaches with the power of DL has opened new avenues for understanding the complexity of DNA methylation and its implications in human diseases. As genome-wide DNA methylation profiling becomes more accessible, the application of DL in this field is expected to enhance further our understanding of epigenetic regulation and its potential clinical applications.

DL researchers can collect epigenomic data from single or multiple sources, and two of the most common public databases are The Cancer Genome Atlas (TCGA) and the Gene Expression Omnibus (GEO).

TCGA was established through a joint effort of the National Cancer Institute (NCI) and the National Human Genome Research Institute (NHGRI) to generate comprehensive, multidimensional maps of genomic changes from over 11,000 cancer cases across 33 cancer types. The TCGA database offers a vast amount of DNA methylation and RNA-seq data accessible to researchers within the cancer research community through the Genomic Data Commons data portal TCGA provides data at different levels of processing: level 1 indicates raw and un-normalized data, level 2 indicates normalized and/or intermediately processed data, level 3 indicates integrated, normalized, and/or segmented data, and level 4 refers to results of integrative or pan-cancer analyses. Among these, level 1 data make up the majority.

GEO, launched in 2000 by the National Center for Biotechnology Information (NCBI), is an international public repository for high-throughput genomic datasets. It accepts both raw and processed data generated using various technologies, including DNA microarrays, high-throughput nucleic acid sequencing, protein or tissue arrays, serial analysis of gene expression, and reverse transcription polymerase chain reaction. While approximately 90% of the data in GEO are gene expression data, it also contains comprehensive datasets for DNA methylation, RNA-seq, and other omics data types [18]. The workflow for developing a predictive model was presented in Figure 2.



**Figure 2.** A workflow for developing a predictive model in translational epigenomics.

Processing raw epigenomic data for analysis involves specific steps tailored to the data's nature. Here's a flow for raw data processing in the context of epigenomic data:

**Importing Data:** Put the unprocessed epigenomic data into your programming suite. Such data may include information from multiple epigenetic assays, including ATAC-seq, DNA methylation, and ChIP-seq.

**Summarizing and Visualizing Raw Data:** Examine the data types and dimensions to gain an understanding of the data's structure. To understand the data distribution, summarize

the fundamental statistics. To see trends and possible problems, visualize the data with plots and graphs.

**Data Cleaning:** Eliminate any noisy or unnecessary data that could interfere with the analysis. This could entail eliminating duplicate data, processing data from batch effects if relevant, or filtering out low-quality or low-confidence data points.

**Handling Missing Values:** For a variety of reasons, including technological constraints or experimental errors, epigenomic data sometimes contains missing values. Select suitable imputation techniques to complete missing values without skewing the data.

**Normalization:** Adjust the data to account for biases introduced during data production or variations in sequencing depth. Total read count normalization, RPKM (Reads Per Kilobase per Million mapped reads), and TPM (Transcripts Per Million) are common normalization methods for epigenomic data.

**Dimensionality Reduction:** High-dimensional epigenomic datasets may lead to overfitting and other computational difficulties. Reduce the number of features while maintaining the underlying structure using dimensionality reduction techniques such as Principal Component Analysis (PCA) or t-distributed Stochastic Neighbor Embedding (t-SNE).

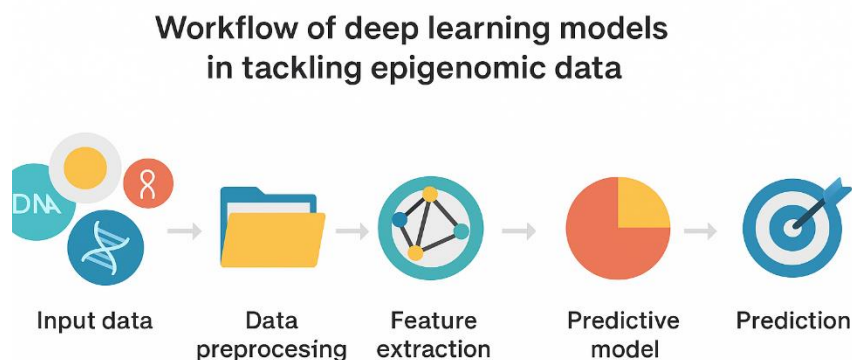
**Feature Selection:** Choose informative features that are pertinent to the particular analysis or prediction task. Differential analysis and statistical testing are examples of feature selection approaches that can be used to identify epigenetic traits associated with various conditions or outcomes.

**Handling Outliers:** Find and deal with any data outliers. A number of factors, such as genuine biological differences or technical errors, might cause outliers in epigenomic data. You may decide to apply the proper adjustments or eliminate outliers, depending on the circumstances.

**Train-Validation-Test Split:** Divide the previously processed data into test, validation, and training sets. This is necessary for training the deep learning model, adjusting hyperparameters, and evaluating performance on unknown data.

**Interpretation and Validation:** Interpret the results to determine which features are essential for analysis or prediction once the deep learning model has been trained on epigenomic data. To make sure the model is generalizable, validate its performance on separate test datasets.

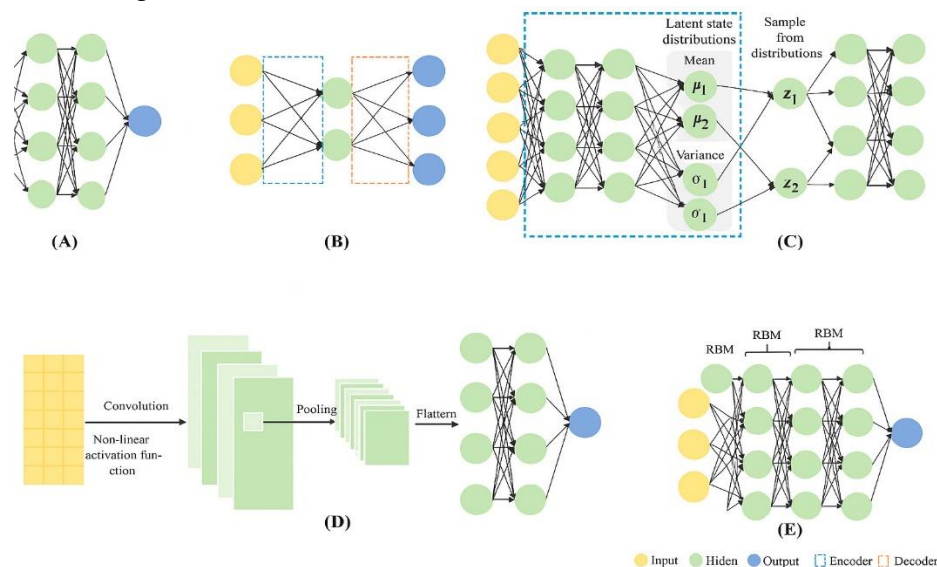
Data preprocessing flow for developing a predictive model in epigenomics was shown in Figure 3.



**Figure 3.** Workflow of DL models in tackling epigenomic data and developing a predictive model in epigenomics.

3.4. Network architectures.

That's a correct description of Artificial Neural Networks (ANNs) and Deep Neural Networks (DNNs). Let's break it down further. Artificial Neural Networks (ANNs): An ANN is a computational model inspired by the structure and functioning of the human brain. It consists of nodes (neurons) organized into layers. The layers are connected through weighted connections. The first layer is the input layer, the last layer is the output layer, and any layers in between are referred to as hidden layers. Information flows forward through the network, from the input layer to the output layer, passing through the hidden layers. Weight Optimization: During training, the network learns to adjust the weights of its connections between neurons to minimize the difference between predicted outputs and ground truth (target) values. This optimization process is typically achieved using gradient descent algorithms like backpropagation. Deep Neural Networks (DNNs): A DNN is a specific type of ANN that consists of multiple hidden layers, making it "deep." These hidden layers enable the network to learn complex representations and patterns in the data. Each hidden layer contains computational units (neurons) that process data from the previous layer and pass their results to the next layer. The presence of multiple hidden layers enables DNNs to handle more complex tasks and extract hierarchical features from data. Epigenomics and DNNs: DNNs have been widely applied in the field of epigenomics to address various human disease-related tasks. The study of genome alterations that do not result from mutations to the underlying DNA sequence is known as epigenomics. This covers chromatin accessibility, histone modifications, DNA methylation, and other things. DNNs have shown promise in tasks such as predicting gene expression levels based on epigenetic marks, identifying disease-associated epigenetic patterns, and interpreting regulatory elements in the genome. By leveraging the power of DNNs, researchers can effectively process and analyze large-scale epigenomic data, leading to better insights into the role of epigenetics in human diseases and other biological processes. However, working with DNNs also requires careful consideration of data preprocessing, model architecture, hyperparameter tuning, and validation to achieve reliable and meaningful results. DL architectures applied in epigenomics to address human disease-related prediction tasks were presented in Figure 4.



**Figure 4.** DL architectures that have been applied in epigenomics to solve some human disease-related prediction tasks. (A) Multi-layer perceptron; (B) Autoencoder; (C) Variational autoencoder; (D) Convolutional neural network; (E) Deep belief network.

## **4. Conclusion**

In conclusion, the article provides a comprehensive review of 22 Deep Learning (DL) based predictive models for various tasks in human disease detection, subtype classification, and treatment response prediction using epigenomic data. The review offers valuable insights into prediction tasks, data types, data sources, neural network architectures, model structures, and prediction performance, making it a valuable resource for researchers looking to develop or enhance their models. The review highlights the superiority of DL models over traditional Machine Learning (ML) models, indicating their potential applicability in clinical settings in the future. DL models have demonstrated impressive performance in analyzing epigenomic data and extracting valuable insights for disease-related tasks. However, the article also points out some challenges that need to be addressed. One significant challenge is the lack of validation and replication of predictive models. By shedding light on the current state of DL applications in epigenomics and addressing their limitations, this review serves as a bridge between DL and epigenomics. It can encourage researchers to collaborate and work towards the advancement of DL models in translational epigenomics, leading to improved clinical applications and furthering our understanding of the epigenetic basis of human diseases. Overall, the article provides a valuable resource for researchers in the field and, by addressing the identified challenges, DL can make significant contributions to epigenomics in the future.

## **Author Contributions**

Conceptualization, R.K.G. and S.V.R.; methodology, R.K.G. and G.K.H.; software, R.K.G.; validation, P.D.P., G.K.H., and R.K.G.; formal analysis, S.V.R.; investigation, R.K.G.; resources, R.K.G., S.V.R.; data curation, G.K.H.; writing—S.V.R, X.X.; writing—review and editing, R.K.G.; visualization, S.V.R, R.K.G.; supervision, G.K.H., P.D.P. All authors have read and agreed to the published version of the manuscript.

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## **Conflicts of Interest**

The authors declare no conflict of interest.

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