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Radiomics and Transformer-Based Deep Learning for Non-Invasive Prediction of PD-L1 Expression in Non-Small Cell Lung Cancer: A Paradigm Shift in Precision Oncology

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Traditional biomarker testing for Programmed Death-Ligand 1 (PD-L1) in Non-Small Cell Lung Cancer (NSCLC) remains invasive and costly. This study proposes a non-invasive alternative by integrating radiomic features extracted from CT scans with advanced deep learning architectures. We evaluated Artificial Neural Networks (ANN), Convolutional Neural Networks (CNN), and Recurrent Neural Networks (RNN), including Long Short-Term Memory (LSTM) and Gated Recurrent Units (GRU). Our results demonstrate that Transformer-based models significantly outperform conventional approaches, achieving a test Mean Squared Error (MSE) of 18.25 compared to 294.59 for ANN and 127.12 for CNN. The optimized Complex Transformer architecture reduced MSE to 17.41 after 1000 epochs, with early stopping at epoch 261. These findings highlight the potential of radiomics combined with Transformer models to enable accurate, cost-effective PD-L1 prediction, advancing personalized oncology while reducing reliance on invasive procedures.

Keywords: *radiomics; deep learning; PD-L1 biomarker; non-invasive diagnostics; non-small cell lung cancer; transformer models.*

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1. Introduction

Non-Small Cell Lung Cancer (NSCLC), a predominant contributor to global cancer mortality, underscores the urgent need for innovations in precision oncology. Central to this pursuit are biomarkers like Programmed Death-Ligand 1 (PDL1), which guide immunotherapy selection and optimize therapeutic outcomes [1]. Traditional approaches for biomarker assessment – invasive tissue biopsies and molecular analyses – impose significant burdens on patients, both financially (costing hundreds to thousands of dollars per test) and physically [1]. Concurrently, routine imaging modalities such as Computed Tomography (CT), Positron Emission Tomography (PET), and Magnetic Resonance Imaging (MRI), while indispensable for diagnosis, amplify healthcare expenses, with individual scans ranging from 1 000 to 5 000 [2]. These challenges highlight a critical demand for cost-effective, patient-centric alternatives.

Radiomics, a transformative field that converts medical imaging data into quantitative biomarkers, offers a paradigm shift. Emerging evidence demonstrates its capacity to predict PDL1 expression non-invasively by integrating radiomic features with deep learning algorithms, thereby circumventing the limitations of tissue-based methods [1, 3]. Such advancements hold promise for reducing diagnostic costs, minimizing patient discomfort, and accelerating treatment planning [4]. For instance, recent studies leveraging CT and PET/CT scans have achieved notable accuracy in PDL1 prediction (AUC: 0.85–0.93), validating radiomics as a viable adjunct to conventional testing [1, 3].

Despite these strides, the clinical integration of radiomics and artificial intelligence (AI) faces hurdles. Robust implementation demands access to large, annotated datasets, sophisticated computational infrastructure, and advanced machine learning frameworks to ensure reliable feature extraction and model generalizability [5]. Nevertheless, the potential rewards are profound: AI-driven radiomics could redefine NSCLC management by enabling real-time, non-invasive biomarker profiling, thereby enhancing therapeutic precision while alleviating healthcare costs [2].

This study investigates the predictive efficacy of radiomic features for PDL1 expression in NSCLC through a systematic comparison of machine learning and deep learning models. By evaluating their performance across diverse datasets, we aim to establish a foundation for integrating AI-powered radiomics into clinical workflows, ultimately bridging the gap between imaging data and molecular diagnostics.

2. Related work

The convergence of radiomics and deep learning has emerged as a transformative force in non-small cell lung cancer (NSCLC) research, offering unprecedented opportunities for non-invasive biomarker prediction and treatment personalization. By extracting high-dimensional data from medical imaging, radiomics enables the identification of latent patterns correlated with molecular features, clinical outcomes, and therapeutic responses [4]. This section synthesizes recent advancements, challenges, and future directions in this rapidly evolving field.

Programmed Death-Ligand 1 (PDL1), a critical biomarker for immune checkpoint inhibitor eligibility, has been a focal point of radiomics research. Traditional tissue-based PDL1 assessment faces limitations due to tumor heterogeneity and invasiveness. Recent studies demonstrate that radiomic features derived from CT and PET/CT scans, when integrated with deep learning models, achieve high predictive accuracy (AUC: 0.85–0.93) for PDL1 expression [1,3]. For instance, Zhang et al. developed a hybrid framework combining radiomics and convolutional neural networks (CNNs), achieving robust performance across multicenter cohorts [2]. These approaches not only circumvent biopsy-related risks but also reduce diagnostic costs by leveraging routinely acquired imaging data.

Epidermal Growth Factor Receptor (EGFR) mutations, pivotal for tyrosine kinase inhibitor (TKI) therapy, have similarly benefited from radiomic innovations. Wang et al. pioneered a multitask AI system using CT-based radiomics to concurrently predict EGFR and PDL1 status, achieving AUCs of 0.928 and 0.905, respectively [6]. Building on this, Wu et al. introduced a habitat radiomics nomogram incorporating peritumoral features, which demonstrated strong generalizability across external validation cohorts (AUC: 0.809–0.917) [7]. Such models exemplify the potential of radiomics to guide targeted therapy decisions non-invasively.

Recent efforts have expanded radiomics to encompass immune-related biomarkers like tumor mutation burden (TMB) and composite prognostic models. Shi et al. developed a radiomic signature integrating PDL1 and TMB data, achieving 83% accuracy in predicting short-term immunotherapy response [8]. Similarly, Sui et al. established a radiogenomic framework linking CT-derived features with gene expression profiles, enabling bidirectional mapping between imaging phenotypes and molecular alterations [9]. These multimodal approaches provide holistic insights into tumor biology, enhancing precision in treatment stratification.

The shift from handcrafted radiomic features to deep learning-driven feature extraction has markedly improved predictive performance. Whereas traditional radiomics relied on manual feature engineering, CNNs and generative adversarial networks (GANs) now autonomously capture discriminative imaging patterns [5]. For example, Sui et al. employed autoencoders to decode tumor heterogeneity from CT scans, significantly outperforming conventional radiomic models in mutation prediction [9]. These advances underscore deep learning's capacity to uncover complex tumor characteristics invisible to human observers.

Despite its promise, clinical translation of radiomics faces critical hurdles:

— **Technical Variability:** Inconsistent imaging protocols (e.g., slice thickness, scanner vendors) impair feature reproducibility [2].
— **Data Scarcity:** Limited access to large, annotated datasets – particularly for rare subtypes – constrains model generalizability [10].
— **Interpretability Gap:** The "black-box" nature of deep learning models hinders clinical trust. Frameworks linking radiomic features to genomic alterations, as proposed by Sui et al., aim to bridge this gap [9].

The integration of radiomics with multi-omics data (genomics, proteomics) represents the next frontier. Mlynar et al. highlighted the synergistic potential of combining imaging biomarkers with molecular profiles to build robust predictive models [11]. Furthermore, federated learning approaches could address data scarcity by enabling collaborative model training across institutions while preserving patient privacy [12].

Radiomics and deep learning are redefining NSCLC management by enabling non-invasive biomarker prediction and personalized treatment planning. While challenges in standardization and interpretability persist, ongoing methodological innovations – coupled with multimodal data integration – position radiomics as a cornerstone of future oncology practice. As evidenced by recent studies, these technologies not only enhance diagnostic accuracy but also pave the way for cost-effective, patient-centric care paradigms.

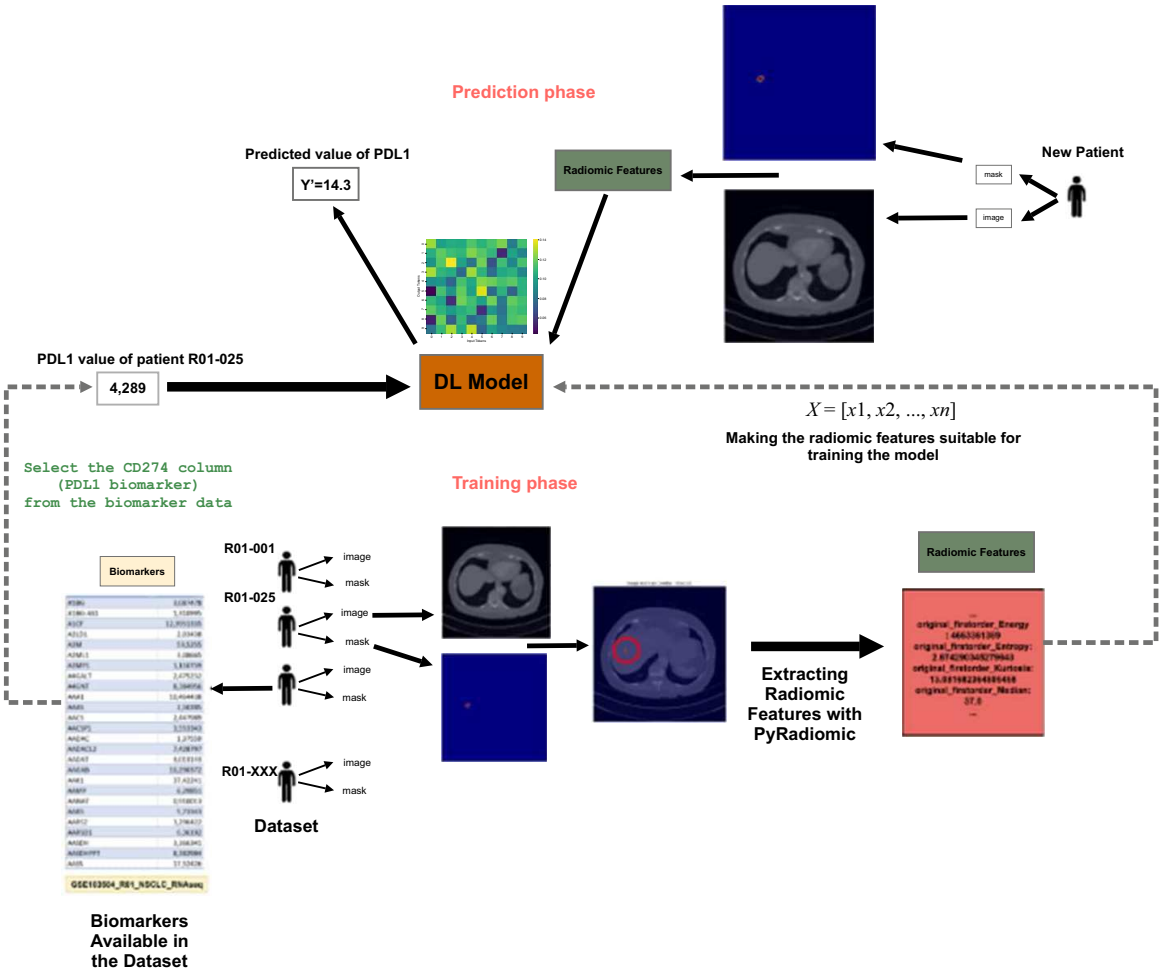

Fig. 1. Overview of the methodology and workflow for radiomic feature extraction and PD-L1 prediction.

3. Proposed methodology

In this study, we aim to predict PD-L1 expression levels in NSCLC patients using a deep learning model trained on radiomic features extracted from CT scans. By combining radiomic data and genomic information, we create a comprehensive framework that allows for the non-invasive prediction of biomarkers critical to patient treatment strategies. The radiomic features, derived from tumor-specific regions in the CT images, capture the tumor's intensity, shape, and texture characteristics, which are key to identifying tumor heterogeneity. These features, alongside corresponding biomarker data, serve as inputs to our deep learning model, which is designed to predict PD-L1 expression levels, aiding in decision-making for immunotherapy treatments.

3.1. Dataset

This study used the NSCLC Radiogenomics Dataset [10] from The Cancer Imaging Archive (TCIA), which includes over 300 patient cases and approximately 30.7 GB of data across 39 626 files and 442 folders. The dataset provides CT images, tumor-specific segmentation masks, and biomarker information like PD-L1 expression levels, crucial for precise radiomic feature extraction. Despite its strengths, variability in imaging protocols and patient demographics presents challenges, highlighting the need for rigorous standardization during preprocessing. This dataset serves as a robust foundation for integrating imaging and genomic data to advance non-invasive cancer diagnostics.

3.2. Data preprocessing

For this study, we selected CT scans and their corresponding segmentation masks for each patient from the NSCLC Radiogenomics dataset. The images underwent preprocessing to standardize resolution and format across the dataset. Scans that lacked corresponding segmentation masks, or images that did not align with their masks in terms of shape, were excluded. This step was essential for ensuring that only valid image-mask pairs were used for further analysis.

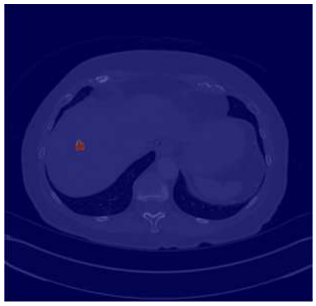

Fig. 2. Image and mask overlap.

The segmentation masks provided in this dataset were manually annotated, allowing precise delineation of tumor regions in the CT scans (Figure 2). This enabled the isolation of tumor-specific features in the volumetric images (Figure 3). Additionally, only CT images (identified by the modality field in the metadata) were included, while scans from other modalities, such as PET or MRI, were excluded. To further examine the data, each CT scan was viewed with its overlaid mask across the axial, sagittal, and coronal planes (Figures 4 and 5). These steps ensured consistency in the dataset used for radiomic feature extraction and subsequent model training.

Fig. 3. Grid view of slices, overlying mask with image.

For the biomarker data, missing PD-L1 values were imputed using the median PD-L1 value across all patients, ensuring no patient data was excluded due to incomplete biomarker information.

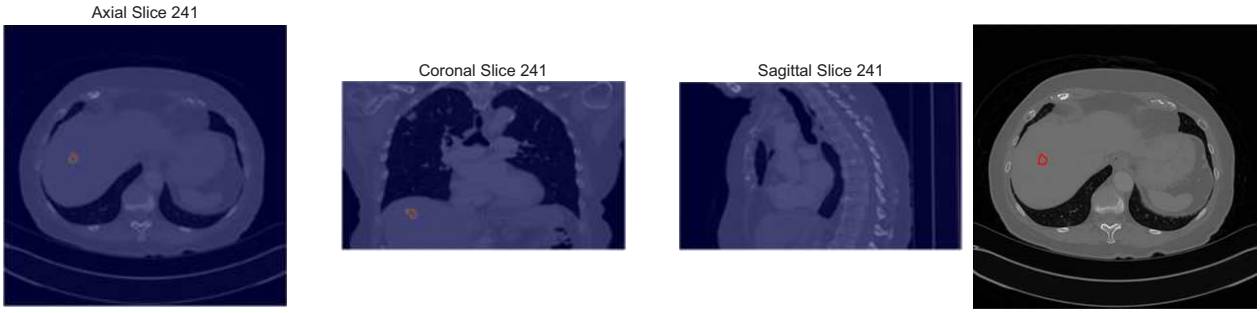

Fig. 4. Views of the overlying mask with image in slice 241 in a patient.

Fig. 5. Image and mask contour.

3.3. Feature extraction

Radiomic feature extraction was performed using PyRadiomics [12], a widely-used open-source library. This library automates the extraction of various quantitative features from the segmented regions of interest (ROIs) within the CT scans. The extracted features include:

- **First-order statistics:** Metrics like mean, median, skewness, and kurtosis, which provide basic intensity information.
- **Shape-based features:** Characteristics of the tumor's 2D/3D structure, such as volume, surface area, and compactness.
- **Texture-based features:** Metrics like the Gray Level Co-occurrence Matrix (GLCM), Gray Level Run Length Matrix (GLRLM), and Gray Level Size Zone Matrix (GLSZM), which provide information on the heterogeneity of the tumor's texture.

After extraction, the features were standardized using z-score normalization to ensure they all contributed equally during model training. Only patients with matching imaging and genomic data were included, ensuring a robust and consistent dataset.

3.4. Deep learning models

In this study, several deep learning architectures were evaluated for predicting PD-L1 expression, each offering unique strengths in processing the complex radiomic features of tumor images:

- **Artificial Neural Networks (ANN):** Basic models with layers of neurons that transform input data to make predictions, useful for identifying general patterns.
- **Convolutional Neural Networks (CNN):** Effective for spatial data, capturing complex patterns in radiomic features by processing data in 2D arrays.
- **Recurrent Neural Networks (RNN):** Capture sequential dependencies, here applied to analyze relationships across tumor layers.
- **Long Short-Term Memory (LSTM):** An RNN variant that better retains long-term information, helping capture changes across multiple tumor layers.
- **Gated Recurrent Units (GRU):** A simpler, faster RNN that handles sequential data efficiently.
- **Transformer Model:** Uses self-attention to weigh feature importance, excelling at identifying complex dependencies in high-dimensional radiomic data.

Each model adds unique strengths, enhancing predictive accuracy for PD-L1 expression.

Hyperparameter tuning. To optimize the performance of the models, hyperparameter tuning was performed using a grid search method.

The following hyperparameters were tuned:

- **Learning Rate:** Adjusting the step size at each iteration while moving toward the minimum of the loss function.

— **Number of Layers:** Exploring the depth of the network by adjusting the number of hidden layers in the models.
— **Number of Neurons per layer:** Modifying the number of neurons within each hidden layer.
— **Batch Size:** Determining the number of samples processed before updating the model's weights.
— **Dropout Rates:** Introducing dropout to prevent overfitting by randomly dropping units from the neural network during training.

The best combination of hyperparameters was selected based on minimizing the Mean Squared Error (MSE) and Mean Absolute Error (MAE) on the validation set.

4. Experiments and results

In this section, we detail the results obtained in terms of Mean Squared Error (MSE), Root Mean Squared Error (RMSE), and Mean Absolute Error (MAE). These metrics were used to evaluate the performance of several deep learning models employed for predicting PD-L1 biomarker expression from radiomic features. Our analysis indicates promising results; however, achieving these results was not without challenges. In the next section, we will address several key challenges encountered during this study, including data variability, model training complexities, and the impact of imaging inconsistencies on predictive accuracy. We will discuss the strategies implemented to manage these challenges and their implications for model generalizability and clinical applicability.

4.1. Challenges in data variability and model training

The NSCLC Radiogenomics Dataset posed challenges due to variability in imaging protocols, patient demographics, and scanner characteristics, which impacted model generalization. Data preprocessing techniques like normalization and segmentation standardization were applied, but some variability persisted, affecting model stability and accuracy. Training deep learning models, particularly Transformers, required significant computational resources and careful hyperparameter tuning. Techniques like early stopping and gradient clipping were used to stabilize training, but balancing complex relationships and generalization re-mained challenging.

4.2. Model selection and performance comparison for PD-L1 expression prediction

In the model selection phase, various machine learning and deep learning models were tested to identify the optimal architecture for predicting PD-L1 expression. The models evaluated included ANN, CNN, RNN, LSTM, GRU, and Transformer-based architectures. These models were chosen for their capacity to capture the complexity of radiomic features extracted from the NSCLC Radiogenomics Dataset. Due to the nature of the data and complex relationships between features, attention-based architectures like Transformers were emphasized for their ability to capture intricate dependencies. The dataset was split into training and test sets for a robust evaluation, with early stopping criteria implemented to prevent over-fitting by monitoring validation set performance. MSE, RMSE, and MAE were calculated as performance metrics for each model, aiming to minimize these er-rors for more accurate PD-L1 predictions. As shown in Figure 6, the performance of each model was compared across multiple metrics during both training and testing phases. The Transformer-based model consistently outperformed the others, achieving lower test MSE, RMSE, and MAE values, indicating superior generalization to unseen data. Traditional models like ANN and CNN showed some promise but struggled to maintain accuracy as the feature set complexity increased. The final performance results on the test data are depicted in Figure 7, where error metrics (MSE, RMSE, MAE) are visualized for clearer comparison. The Transformer model demonstrated the lowest errors across all metrics, highlighting its suitability for PD-L1 biomarker prediction, while models like ANN and RNN exhibited significantly higher error rates, particularly in MSE.

4.3. Proposed model: complex transformer model and hyperparameter tuning

We designed a custom Complex Transformer model to capture the complexities of radiomic feature data (Figure 8). The architecture includes multiple transformer encoder layers with attention heads,

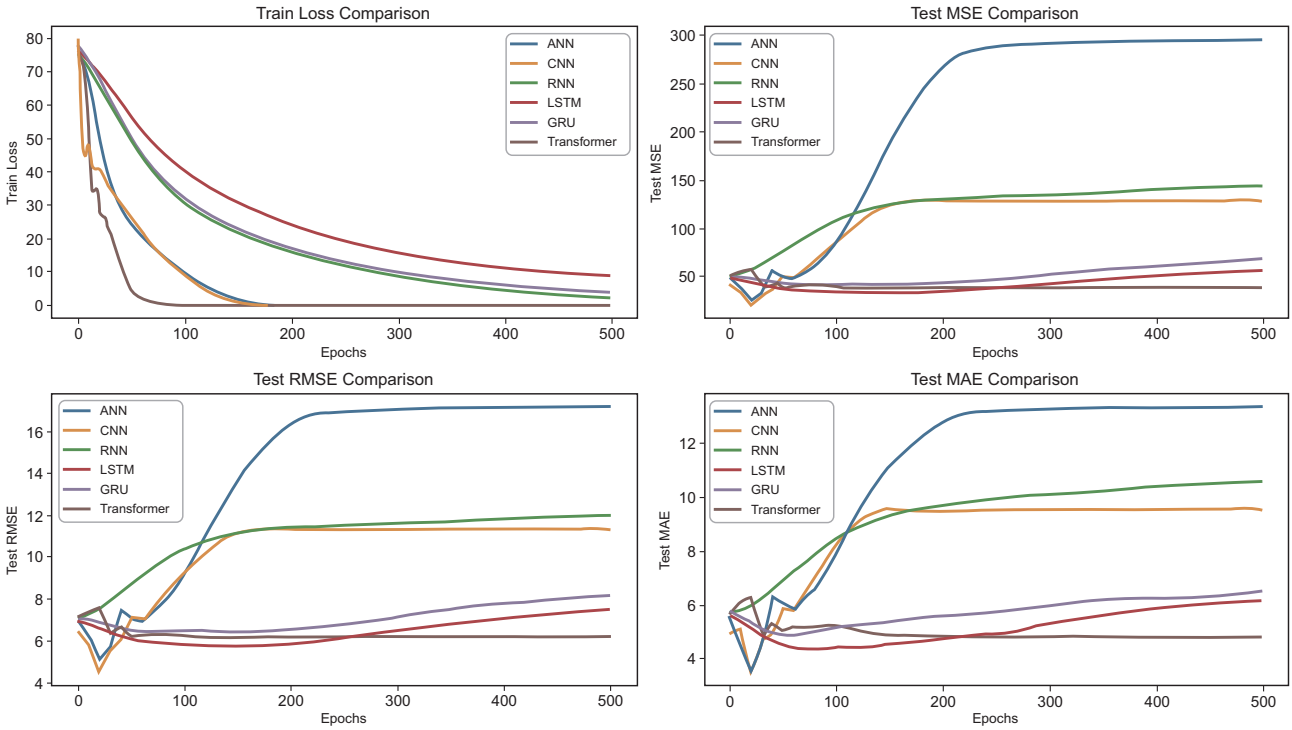

Fig. 6. Performance comparison of used deep learning models over 500 epochs, visualizing Metrics MAE during the model training process.

Fig. 7. Final test results showing the comparison of Metrics for different models.

followed by fully connected layers for refining feature representations. To prevent overfitting, ReLU activations and dropout layers were added. A comprehensive hyperparameter search was conducted, adjusting parameters like learning rate, attention heads, encoder layers, feedforward dimensions, and dropout rate. The optimal configuration included a learning rate of 0.001, 4 attention heads, 6 encoder layers, a feedforward dimension of 1024, and a dropout rate of 0.4. Early stopping at epoch 261 ensured the model's optimal performance for predicting PD-L1 values.

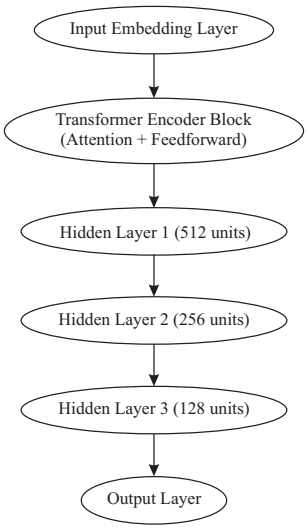

Fig. 8. Architecture of the Complex Transformer Model.

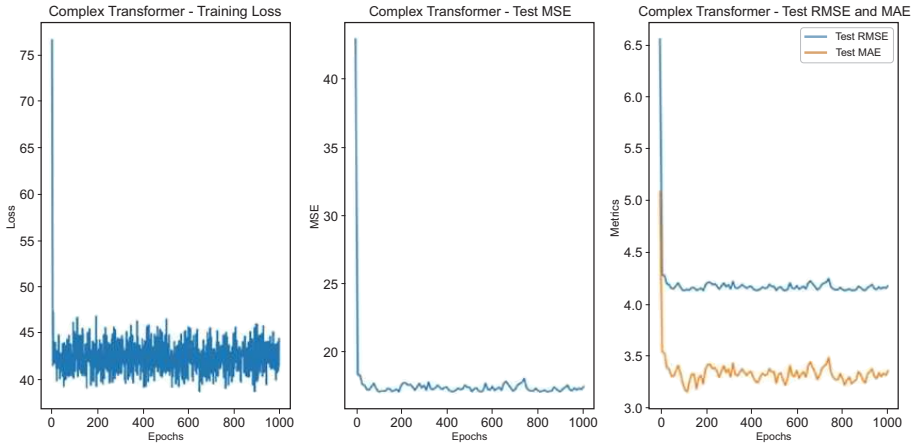

Fig. 9. Training Loss, Test MSE, and Test RMSE/MAE for Complex Transformer Model.

Figure 9 illustrates the training dynamics of the complex Transformer model, showing the training loss, test MSE, and test metrics (RMSE and MAE) over 1000 epochs. The training process highlights stable convergence with early stopping at epoch 261.

Table 1. Complex transformer model performance results.

Model	Epoch Stopped	Final Train Loss	Final Test MSE	Final Test RMSE	Final Test MAE
Complex Transformer	261	44.4359	17.4116	4.1729	3.8041

4.4. Model performance comparison

The comparison illustrated in Figure 10 demonstrates the superior perfor-mance of the Complex Transformer model and its fine-tuned version in comparison to other models such as ANN, CNN, RNN, LSTM, GRU, and the standard Transformer. The Transformer model, along with hyperparameter tuning and early stopping, demonstrated lower MSE, RMSE, and MAE values, as well as a faster convergence rate.

— **Train Loss Comparison**: The Complex Transformer models, especially the Best Complex Transformer with optimized hyperparameters, achieved the lowest training loss across 1000 epochs, demonstrating effective learning without overfitting.
— **Test MSE Comparison**: The Complex Transformer models, particularly the Best Complex Transformer, maintain a consistently low Test MSE throughout training, outperforming models like ANN and RNN and demonstrating superior generalization.
— **Test RMSE and MAE Comparison**: The bottom plots show that the Best Complex Transformer has significantly lower Test RMSE and MAE, maintaining a stable, minimized trajectory, unlike the ANN and CNN models, which show increased error due to poor generalization.

In conclusion, the Complex Transformer and its fine-tuned version demonstrate a substantial improvement in predictive performance, achieving minimal training loss and significantly lower test MSE, RMSE, and MAE compared to all other models. This superior performance emphasizes the effectiveness of attention mechanisms and hyperparameter optimization in handling complex radiomic data for PD-L1 prediction.

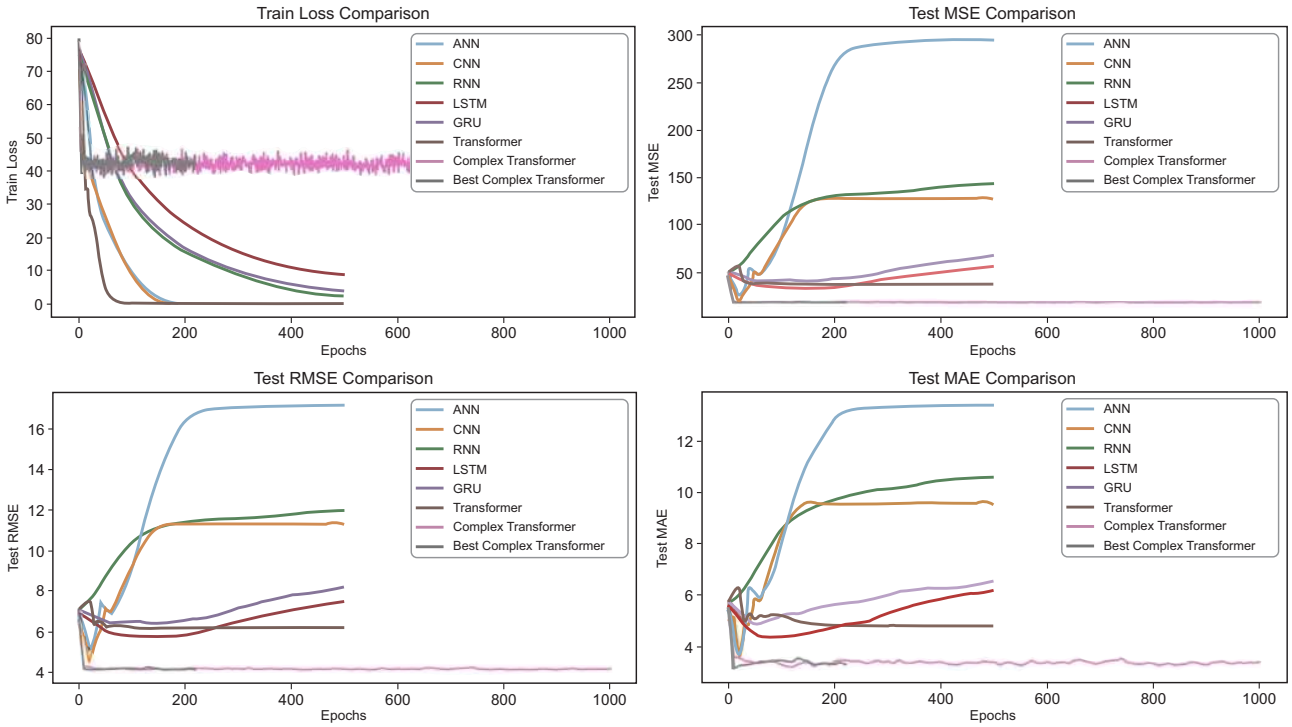

Fig. 10. Model Performance Comparison for Train Loss, Test MSE, and Test RMSE/MAE.

4.5. Clinical relevance and comparative performance of PD-L1 prediction models

For predicting PD-L1 expression, a clinically relevant MSE is typically around or below 20, reflecting accuracy comparable to biopsy results. The Complex Transformer model in this study achieved an MSE of 17.41, showing strong clinical promise and non-invasiveness. It also demonstrated high time efficiency, converging quickly with early stopping at epoch 261. Compared to ANNs and CNNs, which required more epochs and had higher errors, the Transformer's attention mechanisms and interpretability make it especially suited for handling complex radiomic data and supporting clinical decision-making.

4.6. Proposed model performance evaluation

In this section, we provide a detailed technical analysis of our model's performance, focusing on residuals, feature importance, attention mechanisms, and dimensionality reduction, which are critical for evaluating model efficacy.

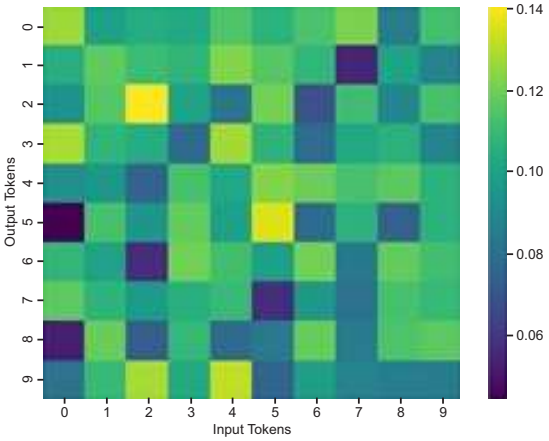

Fig. 11. Attention Weights – Layer.

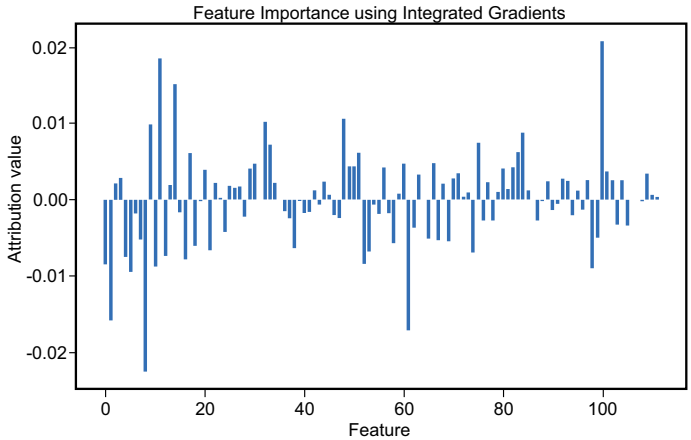

Fig. 12. Feature Importance using Integrated Gradients.

To enhance model interpretability, we analyzed feature importance using Integrated Gradients (Figure 12). This technique measures the contribution of each radiomic feature to predicting PD-L1 values, highlighting features with the most significant positive or negative impact on the model's decisions. Understanding these key features provides insights into the biological and clinical relevance of specific radiomic characteristics, such as tumor texture or shape. Additionally, we explored the attention mechanisms in the Transformer model, which offer transparency by showing how the model allocates focus across input features. The heatmap of Attention Weights in Layer 1 (Figure 11) illustrates the attention distribution across input tokens, helping us identify which aspects of the radiomic data the model considered most important for prediction. This is particularly useful in complex datasets like radiomics, where certain regions of the images may carry more predictive power for PD-L1 expression than others.

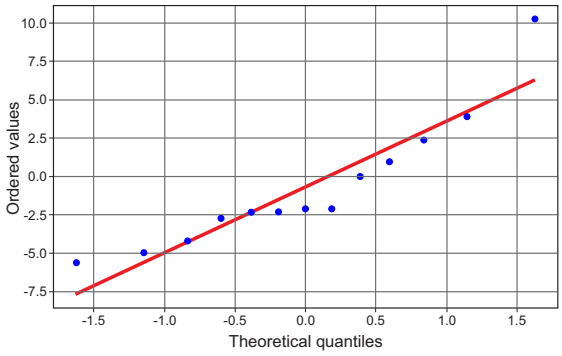

Fig. 13. QQ plot of residuals.

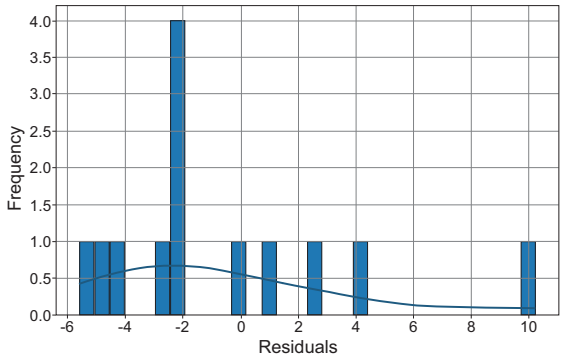

Fig. 14. Residuals distribution.

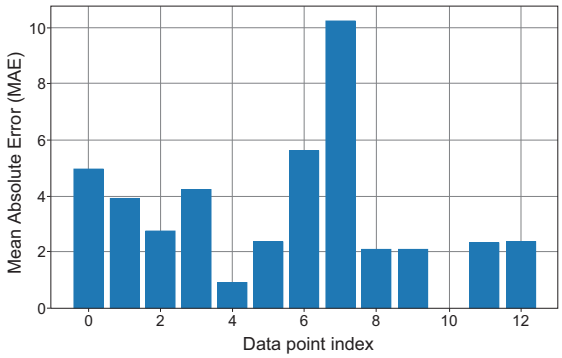

Fig. 15. MAE per data point.

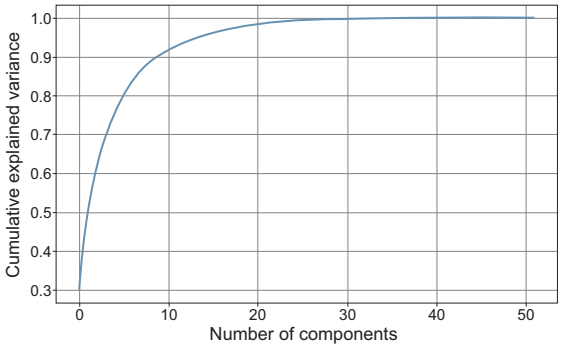

Fig. 16. PCA cumulative explained variance.

We performed a residual analysis to evaluate prediction errors. The Residuals Distribution plot (Figure 13) shows that while the residuals are mostly centered around zero, there is a slight skew, indicating the model has some difficulty predicting PD-L1 values accurately for certain cases. This skew is more pronounced in the Q-Q Plot of Residuals (Figure 14), where deviations from the red line suggest the residuals do not follow a perfect normal distribution. These deviations indicate the model may have struggled with complex relationships in the data, highlighting areas for potential model refinement. Applying Principal Component Analysis (PCA) reduced the radiomic feature space, with the first 10 principal components capturing over 90% of the variance (Figure 15). This dimensionality reduction enhances computational efficiency and accelerates model training while preserving essential predictive information. Additionally, the Mean Absolute Error (MAE) per Data Point plot (Figure 16) reveals high-MAE instances, suggesting outliers or complex cases, aiding in identifying misclassified instances and guiding further model improvement.

4.7. Advantages of the complex transformer architecture

The Complex Transformer architecture with its multi-head self-attention en-hances interpretability and accuracy by focusing on key features, the parallel processing accelerates training and effectively

handles the non-sequential nature of radiomic data. With fine-tuning, the Complex Transformer also showed strong generalization to new data, making it highly suitable for clinical applications that need consistent performance.

4.8. Limitations of the study

Despite its advantages, the study faces several limitations. Variability in radiomic data from different institutions can hinder the model's generalization and accuracy. The sparsity of the matrix, the need for more data, and the high computational requirements of Transformers may also restrict their use in resource-limited settings. The dataset may lack sufficient diversity to fully generalize across broader populations, highlighting the need for larger, more varied samples in future research to enhance robustness and applicability in clinical settings.

5. Conclusion

This study demonstrates that deep learning models, particularly Transformer-based architectures, can effectively predict PD-L1 biomarker expression in NSCLC patients using radiomic data from CT scans. Among tested models (ANN, CNN, RNN, LSTM, GRU, and Transformer), the Complex Transformer with optimized hyperparameters achieved the lowest MSE, RMSE, and MAE, excelling in capturing complex data relationships. Attention mechanisms also identified key features for PD-L1 prediction, highlighting the model's potential to support per-sonalized, non-invasive immunotherapy. Future work may enhance model generalization and address specific data outliers.

Acknowledgments

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Радіоміка та глибоке навчання на основі трансформерів для неінвазивного прогнозування експресії PD-L1 при недрібноклітинному раку легень: зміна парадигми в прецизійній онкології

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Традиційне тестування біомаркера ліганда програмованої смерті 1 (PD-L1) при недрібноклітинному раку легень (НДРЛ) залишається інвазивним і дорогим. Це дослідження пропонує неінвазивну альтернативу шляхом інтеграції радіомних ознак, витягнутих з КТ-сканів, із передовими архітектурами глибокого навчання. Ми оцінили штучні нейронні мережі (ANN), згорткові нейронні мережі (CNN) та рекурентні нейронні мережі (RNN), включаючи довготривалу короткочасну пам'ять (LSTM) та вентильні рекурентні блоки (GRU). Наші результати демонструють, що моделі на основі трансформерів значно перевершують звичайні підходи, досягаючи середньоквадратичної помилки (MSE) тесту в 18.25 порівняно з 294.59 для ANN та 127.12 для CNN. Оптимізована архітектура комплексного трансформера знизила MSE до 17.41 після 1000 епох, із достроковою зупинкою на епосі 261. Ці висновки підкреслюють потенціал радіоміки в поєднанні з моделями-трансформерами для забезпечення точного та економічно ефективного прогнозування PD-L1, сприяючи розвитку персоналізованої онкології та зменшуючи залежність від інвазивних процедур.

Ключові слова: *радіоміка; глибоке навчання; біомаркер PD-L1; неінвазивна діагностика; недрібноклітинний рак легені; моделі-трансформери.*