Impacts of Transformation Techniques and Deep Learning Models on Cell Images Classification Accuracy

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This version was compiled on May 26, 2024

1. Executive Summary

Medical researchers often do not have supporting data to help classify complex large-scale cell images, hence we aim to enhance classification of cell images by gene expression cluster labels, without need for supporting datasets.

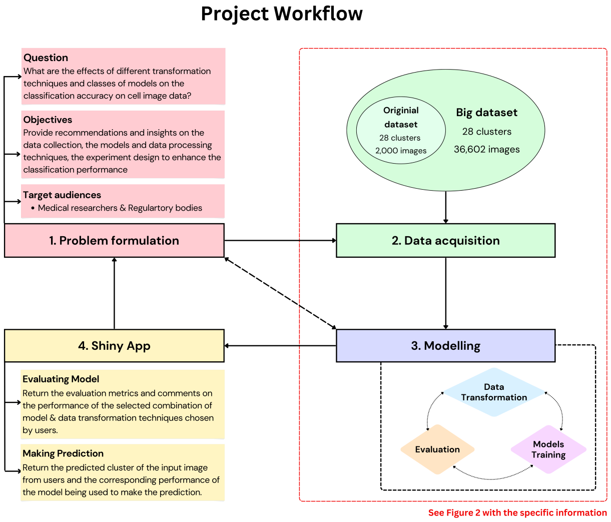
The project found that data augmentation and masking techniques significantly improves the classification accuracy. However, more advanced and deeper networks capture the complex patterns among cell images more efficiently thus having better predicting performance.

Within the report are key figures demonstrating our results with a bar plot on basic CNN performance with data augmentation and masking techniques, a comparative F1 score chart for ResNet18 versus basic CNN across clusters, and an accuracy graph for VIT and transformers across training epochs.

Actionable insights of the impact of data transformations and deep learning models is in the creation of an interactive Shiny platform. The application enables users, likely medical researchers, to upload cell images and receive classifications based on selected models and transformation techniques, translating complex data science processes into actionable insights for users.

2. Introduction

The interpretation and classification of cell images based on gene expression cluster labels play a crucial role in the fields of science and medicine. Cells often exhibit complex phenotypes, such as variations in shape, subcellular protein localization, and other characteristics. The combination of these intricate phenotypic differences and diverse biological responses makes deciphering biological processes increasingly complex (Shifat-E.-Rabbi *et al.*, 2019). Therefore, traditional medical research often struggles with image analysis and prediction due to technical expertise limitations, which is a problem that tends to worsen with increasing data volume and complexity (**?**). To address this issue, the use of advanced computational techniques has become increasingly popular. Computer analysis of cell images can automatically classify cells, providing significant support in scientific, technological, and medical applications. For instance, in pathology, researchers are increasingly exploring methods to automatically detect cancer through cell image classification (Kantara *et al.*, 2015). The aim of this project, therefore, is to investigate the impacts of different data processing techniques and deep learning models on classification performance over cell image data. Our primary focus is on leading medical and biotechnological researchers who need to process large volumes of cell imaging data, and are particularly interested in exploring cellular localisation. To assist these researchers, we introduce a computer vision scheme that accurately identifies cell identities and provides detailed insights into the impact of various data transformations and deep learning models on the classification results (**Figure 1**). This project thus seeks to help researchers gain a deeper understanding of the potential drawbacks associated with their current data collection and experimental design. By providing recommendations and insights, we hope to refine the design and efficiency of cell classification experiments, state-of-the-art methodologies from the data science field, and achieve more accurate results. Given the complexity and pervasiveness of cell images, we decided to focus on deep learning methods, including convolutional neural networks (CNNs) and Transformers, which have emerged as the leading end-to-end classification system (Shifat-E.-Rabbi *et al.*, 2019). Our study also includes various image augmentation techniques to enhance the performance and accuracy of these models. Building on the key findings,we developed an interactive platform - Shiny which will allow users to get insights of models' performance by returning evaluation metrics and detailed description about their selected combination of model and data transformations techniques. The platform also allows users to upload new cell images and select a specific set of model and augmentation techniques to obtain predicted cluster IDs, along with corresponding predicted probability. In creating a user-friendly interface that translates complex data science processes into actionable clear insights visually like Shiny could foster deeper understanding and more effective application of cell image classification techniques.



What are the effects of different transformation techniques and classes of models on the classification accuracy on cell image data?

Provide recommendations and insights on the data collection, the models and data processing techniques, the experiment design to enhance the classification performance

- Medical researchers & Regulartory bodies

Return the evaluation metrics and comments on the performance of the selected combination of model & data transformation techniques chosen by users.

Return the predicted cluster of the input image from users and the corresponding performance of the model being used to make the prediction.

Fig. 1. Workflow

3. Methodology

3.1. Data acquisition. The initial experimentation with the provided images using basic machine learning techniques identified overfitting and low fitting efficiency as significant issues (Appendix). To address these, the project considered an extended training input with transformation techniques (image contour methods) and extended deep learning models. Therefore, the extended image dataset, sourced from the 10X Genomics platform, includes high-resolution cell images, cluster IDs, and cell boundary information from a 10µm section of a C57BL/6 mouse from Charles River Laboratories. The images are stored as lists, with each list representing a grayscale image composed of an array of pixel intensity values. This dataset, comprising 36,602 images across 28 clusters, was subsequently used for further analysis.

3.2. Model development. Based on the reintroduced larger dataset and the problems identified through experiments, it was evident that simple machine learning models and the basic CNN model lacked the necessary complexity. Consequently, our project narrowed its scope to focus solely on deep learning models. ResNet18 and ResNet50 were considered initially, as these mainstream classifiers learn the residual function of the reference layer input, forming a network by stacking residual blocks, their architecture is considered more suitable for optimisation. Beyond CNN models, another main class investigated was Vision Transformers (ViT), which excel in handling large datasets and offer more robust generalisation. The overall deep learning models as shown:

- Basic CNN Model (CNN)
- Resnet 18 (CNN)
- Resnet 50 (CNN)
- ViT (Transformer)

Specifically, the basic CNN model we constructed consists of two convolutional layers with ReLU activation and 2x2 max pooling layers, reducing the input dimensions from 50x50 to 12x12. ResNet18 comprises 18 layers including convolutional, batch normalisation, and identity mapping layers, and ResNet50 consists of 50 layers with a more complex architecture. Different from CNN models, the Vit model (Vit-base) contains 12 layers.

3.3. Transformation and Masking. In addition to efficient models, image augmentation has been proven as an effective and efficient strategy to obtain satisfactory performance with a limited dataset (Xu *et al.*, 2023), which remains as a prevalent obstacle in medical image analysis (Shorten and Khoshgoftaar, 2019). The project thus incorporates several image transformation and masking techniques, including data normalisation and augmentation, with Gaussian filters, Canny contour detection, Sobel edge detection.

Normalisation was applied to the pixel-based data by subtracting the mean of pixel values and dividing by the standard deviation for each image, projecting the pixel values within the predefined range of [0, 1] to ensure consistency within the training input. Image augmentations such as random flipping and random rotation, have been commonly utilised throughout many studies over the last decade for various computer vision tasks such as image classification (Xu *et al.*, 2023), were also implemented with rotating angles ranging from -50 to 50 degrees.

To further enhance model performance, Gaussian blur was implemented by convolving each image with a Gaussian function to smooth the image and reduce noise. This assigns a weight to each pixel based on its distance from the centre, with the blur size set to (25, 25) to specify the kernel size. The convolution operation calculates a weighted average of the surrounding pixel values, reducing high-frequency noise. Additionally, the Canny edge detection method was applied using thresholds of 10 and 200 to detect a wide range of edges by identifying intensity gradients. The final investigation focused on the Sobel edge detector, which performs 2-D spatial gradient measurements on the image to emphasise high spatial frequency regions corresponding to edges. To evaluate the effectiveness of the two transformation, three masking techniques, as well as to identify the most optimal combination with different models, we established the Basic CNN model as our baseline. This decision was made with consideration of the limited computational resources available to the project team.

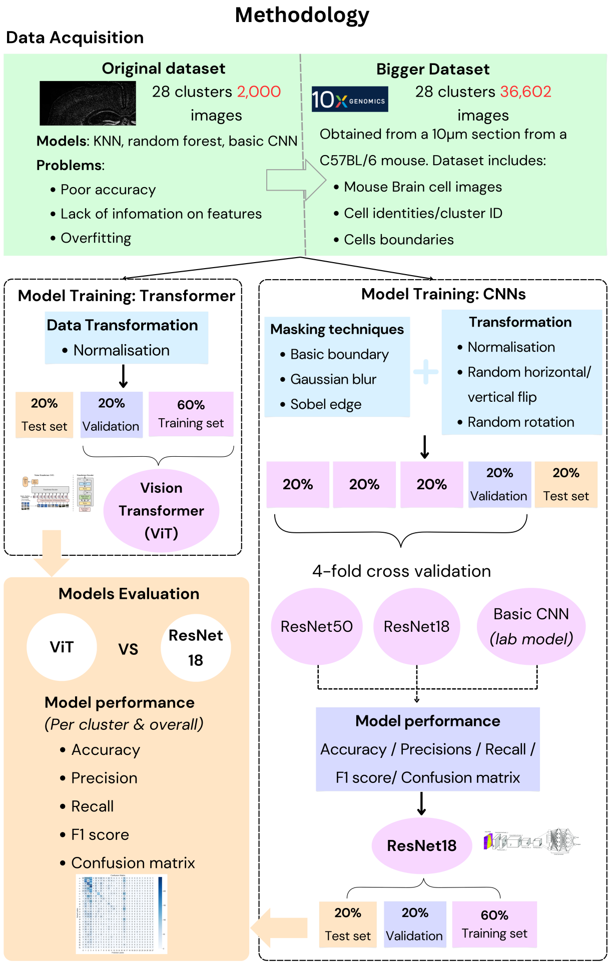


Fig. 2. Methodology

3.4. Training and Validation. The training and validation process began by experimenting with different combinations of transformation techniques on the dataset, which was initially split into 80% training and 20% testing sets. For all of the CNN models, based on 4-fold cross-validation, the training set was further divided into four folds, each containing 20% of the data, and models were trained using these folds. Considering the limitation of computational resources, the ViT model, along with the optimal CNN model, was trained and validated with a single validation set.

During training, instances of overfitting were observed, which were addressed by adding dropout layers to each model. Additionally, the performance of three optimizers—SGD, BGD, and ADAM—was compared, where SGD exhibited noticeable fluctuations, BGD had slow convergence, and ADAM, being relatively robust, was ultimately chosen for all models. Upon completing the training process, the final model's performance was evaluated using the untouched testing set.

3.5. Evaluation strategy. Our evaluation strategies to gauge model performance measured both per-cluster and overall levels. Accuracy serves as the primary indicator of model success, while precision and recall provide more nuanced insights into the model's predictive capabilities, particularly in class imbalances. Precision indicates the proportion of true positive predictions out of all positive predictions made by the model, while recall measures the proportion of true positive cases detected out of all actual positive cases. Generally, precision and recall are inversely related: a more conservative model might have higher precision but lower recall, and vice versa.

To address this, we calculated the F1 score, which balances both precision and recall to provide a single metric that considers both false positives and false negatives. However, we also report precision and recall separately to allow for more specific evaluation scenarios. Furthermore, the confusion matrix further measures model performance by revealing possible patterns of misclassification. To ensure scalability and feasibility for real-world applications, the models are also evaluated in terms of running time and memory usage.

4. Result

4.1. Convolutional Neural Networks (CNNs).

4.1.1. Basic CNN model. Applying image augmentation techniques yields noticeable improvements in the performance of the basic CNN model. Specifically, using the transformed dataset increases 2.6% of accuracy, 3% of precision, and 1 of F1 score than the original one **(Figure 3)**. Normalisation also accounted for most of the results, noticeably doubling the precision. Given the fact that normalisation reduces the differences between the variation range of the different variables, error gradually decreases (Sola and Sevilla, 1997) which improves both convergence and generalisation of the network (Shao *et al.*, 2020).

Image augmentation techniques (random rotation and random flip), except for increasing the accuracy 0.9%, has no impact on the precision and even decreases the F1 score by 1 **(Figure 3)**. As these cells in medical images can appear in many variations, these geometric transformations can introduce variability into the model by changing the perspectives of objects within images mitigating the overfitting issue encountered initially (Xu *et al.*, 2023). However, as both the angle of rotation and axis of flipping directly affect the preservation label identity and variations in the dataset (Xu *et al.*, 2023), the unfavourable outcome might indicate that the chosen magnitude of these operations within this project is not the most optimal one.

All the masking techniques, meanwhile, appear to contribute little to the improvement of model performance. They even worsen the model's accuracy by 0.5 - 0.7% **(Figure 3)**. Although the edge detection and blur type identification techniques have been proven to have remarkable performance on deep learning models (Wang *et al.*, 2017, Guo *et al.* (2021)), the simple architecture of the basic CNN causes its limited capacity and sensitivity to input variations of architecture, which might lead to less capability of benefiting from such complex image preprocessing techniques like masking. The lack of the improvement could indicate that the basic CNN model's architecture is not sophisticated enough to capitalise on the increased variability without additional modification (Tuggener *et al.*, 2022).

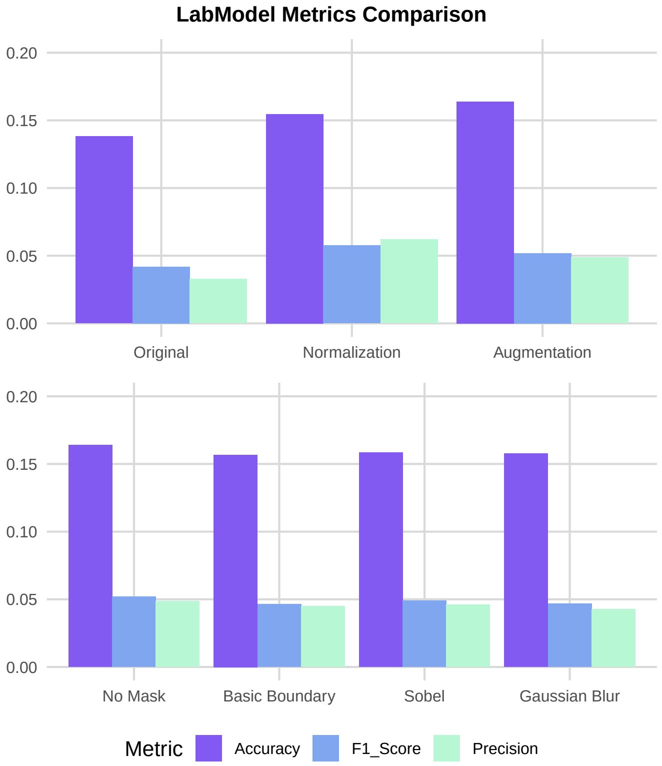


Fig. 3. Basic CNN model under different data transformation and masking techniques

4.1.2. Advanced CNN models (ResNet models). Applying masking techniques on more advanced CNN models shows contrary results, significantly improving the models' accuracy. Specifically, including the cell boundary increases the accuracy by 3.3% on ResNet18 and 2.2% on ResNet50. Using sobel edge adds 4.3% more on the accuracy of ResNet18, and 0.4% for ResNet50. Gaussian blur, which is also the masking technique with best performance on advanced CNNs, better the ResNet18's accuracy by 6.4% and ResNet50 by 5.16% **(Figure 7)**. Given the deeply sophisticated architectures, these two networks appear to gain significant advantages from these advanced image preprocessing methods: masking to better their performance.

4.1.3. Overall CNN models. Comparing the performance of three CNN models over 30 epochs based on the optimal combination (**Figure 8**), the basic CNN model achieved a validation accuracy of 15%, with both training and validation curves remaining smooth. ResNet18 reached a validation accuracy of 17%, stabilizing after initial fluctuations, while ResNet50 achieved approximately 14.5%. None of the models exhibited overfitting, indicating the effectiveness of our preprocessing methods.

Further comparing the F1 scores at the per-cluster level, the ResNet18 model demonstrates superior performance with an average F1 score of 0.09, better than the average F1 score for ResNet50 (0.07) and basic CNN model (0.05) **(Figure 9)**. This indicates that, on average, the ResNet18 balances precision and recall better than others. Specifically **(Figure 4)**, for Cluster 6, ResNet18 achieves an F1 score of 0.45, which matches the performance of the basic CNN. But ResNet18 also outperforms the basic CNN in several other clusters (clusters 2 and 3), by achieving higher F1 scores, indicating its robustness and better generalization capabilities compared to the basic CNN.

Overall, the ResNes18 would be the best model, and as ResNet50 and basic CNN have similar accuracies but better F1-score, we suggest ResNet50 still outperforms basic CNN.

The good performance of ResNet18 can be attributed to its more complex architecture, which includes additional convolutional and pooling operations (Ramzan *et al.*, 2019), allowing it to capture more intricate features compared to the basic CNN model.

Interestingly, ResNet50 did not outperform the basic CNN with its accuracy but the F1-score, in the F1 distribution, while the basic CNN model shows a higher F1 score for certain clusters, both ResNet provide more comprehensive predictions across all clusters. We believed it could be attributed to the observed imbalance in the data, where the basic CNN model's tendency to over-predict certain clusters likely contributed to its seemingly better performance in those specific cases. In addition to this, as the ResNet50 is more complex with the architecture, the lack of performance in ResNet50 compared to ResNet18 might still be due to the model's tendency to over-predict certain clusters for ResNet18. The imbalance issue also leads to its comparable or even lower performance.

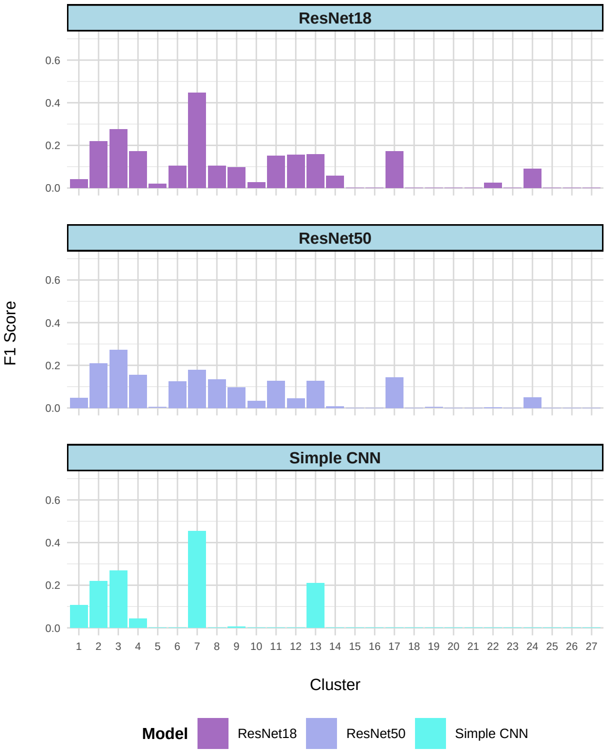


Fig. 4. F1 Scores by Cluster for all Models

4.2. Transformers (ViT).

Under the single validation training **(Figure 5)**, the accuracy of the ViT model increased steadily and continued to grow, while the validation accuracy began to stabilise at around 17.5% after 10 epochs (Figure). In the latter half of the training, we observed signs of overfitting, but the validation curve did not decline significantly, it was considered as a "good" overfitting.

Comparing the single validation training of the best CNN model (ResNet18) **(Figure 5)**, ViT outperformed the CNN by approximately 4% in accuracy. Additionally, ViT made predictions on more clusters (wider prediction) and exhibited higher precision and recall both for each cluster and overall **(Figure 10)**. Therefore, it could be concluded that the ViT model simultaneously satisfies a wide range of predictions and recalls, and demonstrates better performance. This improved performance can be attributed to the generalisation capabilities, the ability to capture global context, combined with its extensive pretraining on large datasets.

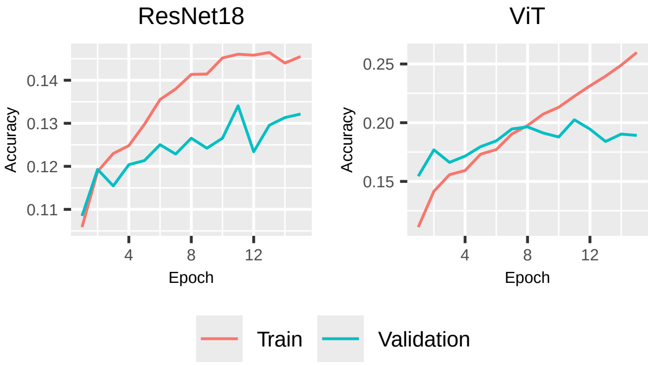


Fig. 5. Train and validation accuracy between ViT and ResNet18

4.3. Shiny.

Key findings are then visualized and presented using an interactive platform Shiny, which enables a more engaging and informative approach to the end-users. The app has three main functions **(Figure 6)**, including:

1. Providing insights of CNNs performance (accuracy, precision, F1 score, etc.). Considering that the dataset has a huge class imbalance problem, Shiny also displays models' performance both overall and across 28 clusters.

2. Providing insights of the Transformers (ViT), with detailed comparison with the best model from CNN class: ResNet18.

3. Predicting clusterID and corresponding predicted probability of cell image uploaded by users, using selected combination of model and data transformation, masking techniques.

4.4. Discussion and Conclusion.

The project findings highlight the importance of selecting appropriate data transformations and model architectures for the task of cell image classification. Normalisation was an universally beneficial preprocessing step, while the effectiveness of image augmentation and masking techniques varied depending on model complexity. The basic CNN model's limitations were highlighted by its inability to benefit from more complex preprocessing methods, whereas advanced CNN models demonstrated significant improvements when these techniques were applied. Overall, ViT appears as the best model with highest prediction performance.

However, it is critical to acknowledge that the success of deep learning in vision depends on three factors: high capacity models, computational power, and availability of large-scale labelled data (Sun *et al.*, 2017). The project's scope and methodology still has several limitations. Specifically, the small dataset size constrained the complexity of the models that could be trained, as more sophisticated models require larger datasets to be effective. The significant imbalance issue across clusters might also potentially introduce certain biases into the models. Additionally, the vague nature of the cluster labels posed a challenge for model interpretability, making it difficult to understand the basis for the model's predictions. Other shortcomings, such as the low model complexity due to limited computing resources and the lack of interpretability, highlight areas for future work to improve the methodology approach.

Therefore, future work can leverage more data from under-represented classes to address the class imbalance issues such as a dataset including the full brain to provide a richer and more varied set of images for analysis. More advanced and deeper network architectures should also be considered for better prediction given the complexity of medical visuals such as cell images. Given that ViT outperforms all CNNs being considered, more networks from this class can be trained to investigate the efficiency of Transformers in medical image analysis. Additionally, the application of cross-validation (CV) across all models would ensure a more robust evaluation of their performance.

Group Contribution

Parth Bhargava (510401900): Converted the Imaging lab set up code from R to Python. Trained some basic CNNs (with J). Worked on Shiny's backend: matched the project's result with the UI's design of models' performance, Image prediction tab. Generated some plots for the final report. Structurised and arranged the group's GitHub repository.

MiaoMiao Chen (520181814): Initial exploration with three masking techniques, the initial ResNet50 model, the basic machine learning models with Hazel, workflow figure, the Methodology figures (with Hazel), part of Shiny design, part of script, part of presentation slides, responsible for the meeting minutes submission, report's methodology, second half of report's results,report formatting in r.

Ethan Chang (520406670): I took notes during workshops and consultations, refined and created slides based on tutor feedback, helped with initial lab model transformations, and improved the presentation script for clarity and flow, ensuring it stayed within the time limit. I created the report abstract, co-wrote the executive summary and improved phrasing.

Hazel Nguyen (510652339): Fitting KNN, Random Forest (with Miaomiao). Two main figures: Workflow & Methodology (with Miaomiao). Part of the Shiny's UI design. Presentation slides (including recorded video of Shiny) and part of the script. Report template and rendering using R's pinp, first half of the report's result, part of the discussion and conclusion.

Evan Nguyen (500469361): I was responsible for writing and editing the report and the presentation script. Additionally I also helped with initial data exploration and assisted with looking into some basic transformation techniques for cells.

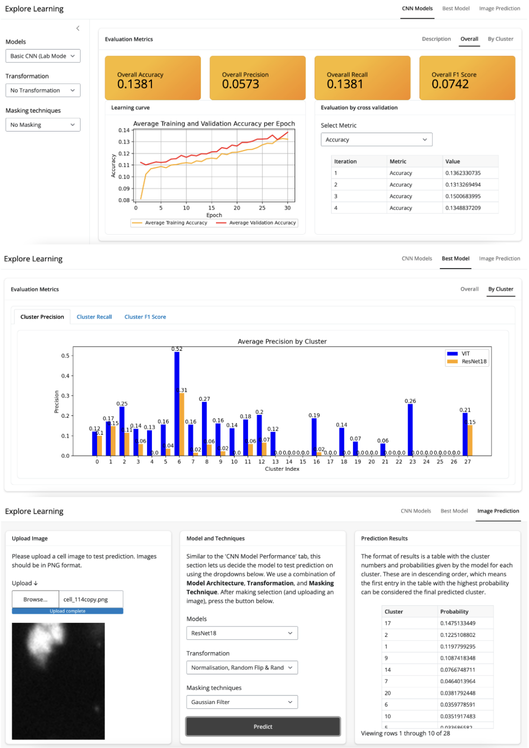
Jiacheng Yu (510050786): I primarily managed the architecture and most of the fine-tuning and training process for deep learning models, concluded save and visualization. Moreover, I explored the shiny app for Python. and built the code architecture for the whole project. Also, I drew about half of the diagrams in the final report.

5. Github and Shiny Link

https://github.com/jiyu4399/DATA3888_Image_Group_2

https://gitparth12.shinyapps.io/data3888_imaging_021/

6. Appendix



Iteration	Metric	Value
1	Accuracy	0.1362330735
2	Accuracy	0.1313269494
3	Accuracy	0.1500683995
4	Accuracy	0.1348837209

Please upload a cell image to test prediction. Images should be in PNG format.

Similar to the 'CNN Model Performance' tab, this section lets us decide the model to test prediction on using the dropdowns below. We use a combination of **Model Architecture**, **Transformation**, and **Masking Technique**. After making selection (and uploading an image), press the button below.

Models: ResNet18

Transformation: Normalisation, Random Flip & Rand

Masking techniques: Gaussian Filter

The format of results is a table with the cluster numbers and probabilities given by the model for each cluster. These are in descending order, which means the first entry in the table with the highest probability can be considered the final predicted cluster.

Cluster	Probability
17	0.1475133449
2	0.1225108802
1	0.1197799295
9	0.1087418348
14	0.0766748711
7	0.0464013964
20	0.0381792448
6	0.0359778591
10	0.0351917483
5	0.033686582

Viewing rows 1 through 10 of 28

Fig. 6. Shiny

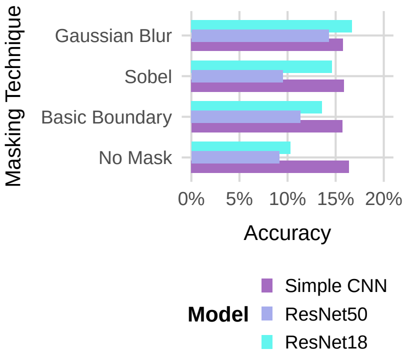


Fig. 7. Models accuracy under different masking techniques

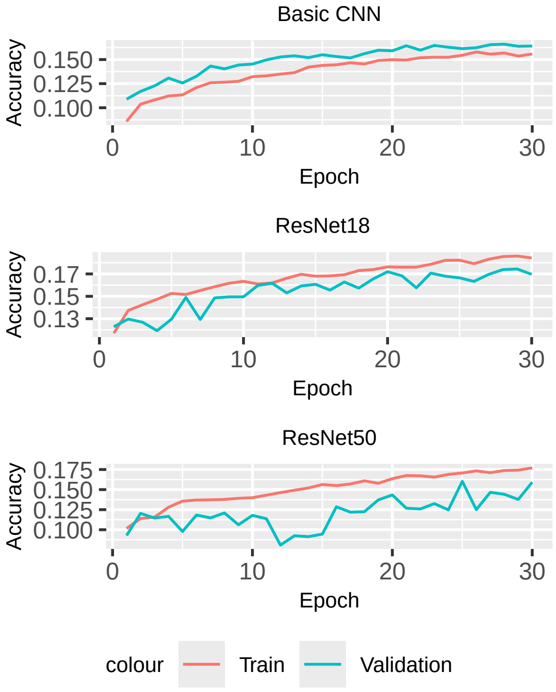


Fig. 8. Train and validation accuracy for all models

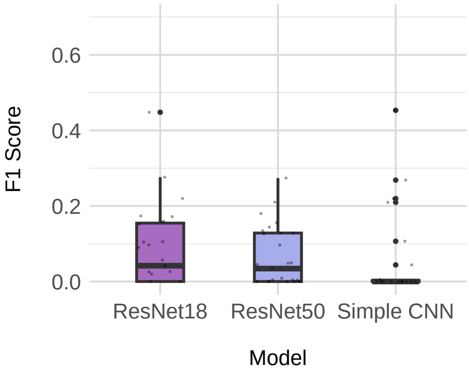


Fig. 9. Average F1 Score Distribution for all models

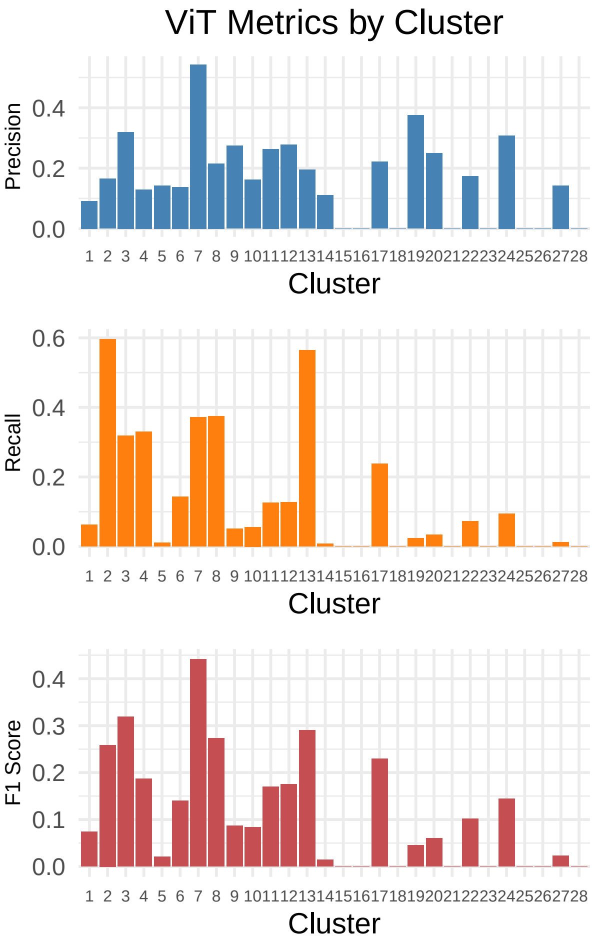


Fig. 10. F1 score per cluster for Vit

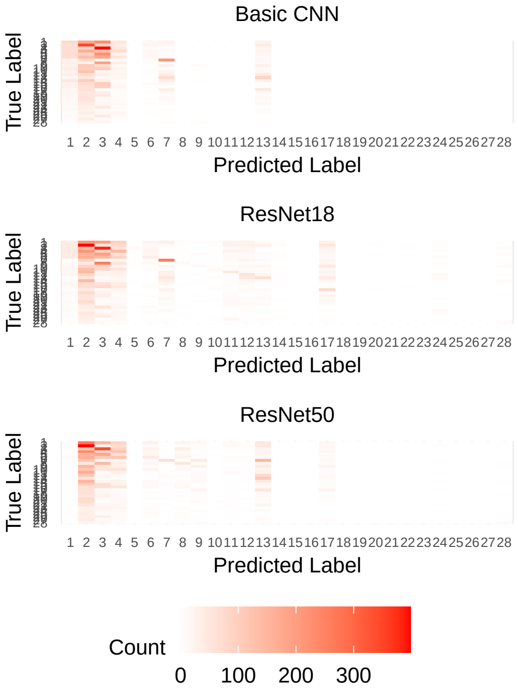


Fig. 11. confusion matrix

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