SaiDL Assignment

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1 CoreML

1.1 Introduction

Label noise presents a significant challenge in supervised learning, potentially leading to overfitting and poor generalization. Traditional loss functions like Cross-Entropy (CE) are particularly susceptible to memorizing noisy labels. This project investigates normalized loss functions and the Active-Passive Loss (APL) framework as solutions, implementing them in PyTorch and evaluating their robustness on the CIFAR-10 dataset with various noise levels.

Prior to this project, my experience in deep learning was limited to Andrew Ng's Machine Learning Specialization and partial completion of his Deep Learning Specialization. This implementation represented a significant step forward in practical application of these concepts.

The paper that forms the theoretical foundation for this implementation proposes that normalizing loss functions can enhance robustness by constraining the loss values within a bounded range, preventing any single example from dominating the gradient updates. While effective for noise robustness, these normalized losses can suffer from underfitting on clean data. The APL framework addresses this limitation by combining the strengths of different loss types.

1.2 Theoretical Background

1.2.1 Loss Functions for Classification

The standard Cross-Entropy (CE) loss for a classification task is defined as:

$$\mathcal{L}_{CE}(x, y) = -\log\left(\frac{e^{x_y}}{\sum_{j=1}^{C} e^{x_j}}\right) = -\log(p_y) \tag{1}$$

where x is the logit vector output from the model, y is the true class, and p_y is the predicted probability for class y.

Focal Loss (FL) extends CE by adding a weighting factor $(1 - p_y)^\gamma$ that reduces the relative loss for well-classified examples:

$$\mathcal{L}_{FL}(x, y) = -(1 - p_y)^\gamma \log(p_y) \tag{2}$$

1.2.2 Normalized Loss Functions

Normalized Cross-Entropy (NCE) divides the CE loss by the sum of negative log probabilities across all classes:

$$\mathcal{L}_{NCE}(x,y) = \frac{-\log(p_y)}{\sum_{j=1}^{C} -\log(p_j)} \tag{3}$$

Similarly, Normalized Focal Loss (NFL) applies the same principle to FL:

$$\mathcal{L}_{NFL}(x,y) = \frac{(1-p_y)^\gamma(-\log(p_y))}{\sum_{j=1}^{C}(1-p_j)^\gamma(-\log(p_j))} \tag{4}$$

This normalization bounds the loss between 0 and 1, making it less sensitive to extreme outliers caused by label noise.

1.2.3 Active-Passive Loss Framework

The APL framework combines two types of losses:

- **Active losses** (e.g., CE, NCE, FL, NFL) that maximize the probability of the true class
- **Passive losses** (e.g., MAE, RCE) that additionally minimize the probabilities of incorrect classes

Mean Absolute Error (MAE) for classification is defined as:

$$\mathcal{L}_{MAE}(x,y) = \frac{1}{C}\sum_{j=1}^{C}|p_j - y_j| \tag{5}$$

where y_j is 1 if $j = y$ and 0 otherwise.

Reverse Cross-Entropy (RCE) is formulated as:

$$\mathcal{L}_{RCE}(x,y) = -A\sum_{j=1}^{C} y_j \log(1-p_j) \tag{6}$$

where A is a negative constant (typically -4).

The APL function combines an active loss $\mathcal{L}_a$ and a passive loss $\mathcal{L}_p$ with weights α and β:

$$\mathcal{L}_{APL}(x,y) = \alpha\mathcal{L}_a(x,y) + \beta\mathcal{L}_p(x,y) \tag{7}$$

1.3 Implementation Details

1.3.1 Data Preparation

The CIFAR-10 dataset, consisting of 60,000 32×32 color images across 10 classes, was used for all experiments. To simulate real-world label corruption, I implemented two noise types:

- **Symmetric noise**: Labels were randomly flipped to any of the other 9 classes with equal probability, using noise rates $\eta \in \{0.2, 0.4, 0.6, 0.8\}$. This was implemented as:

Algorithm 1 Symmetric Noise Generation

```
Input: Labels $Y$, noise rate $\eta$
$\hat{Y} \leftarrow Y$ {Copy original labels}
$indices \leftarrow$ random_permutation(length($Y$))
$noise\_indices \leftarrow indices[0 : \lfloor \eta \times \text{length}(Y) \rfloor]$
for $idx$ in $noise\_indices$ do
  $new\_label \leftarrow$ random_int(0, 9)
  while $new\_label = Y[idx]$ do
    $new\_label \leftarrow$ random_int(0, 9)
  end while
  $\hat{Y}[idx] \leftarrow new\_label$
end for
Return: $\hat{Y}$
```

- **Asymmetric noise (bonus task)**: Labels were flipped to semantically similar classes with probability $\eta \in \{0.1, 0.2, 0.3, 0.4\}$. Specifically:
  - TRUCK $\rightarrow$ AUTOMOBILE
  - BIRD $\rightarrow$ AIRPLANE
  - DEER $\rightarrow$ HORSE
  - CAT $\rightarrow$ DOG
  - DOG $\rightarrow$ CAT

  This simulates more realistic annotation errors where visually similar classes are confused.

Standard data augmentation techniques were applied, including random cropping, horizontal flipping, and normalization with mean $(0.4914, 0.4822, 0.4465)$ and standard deviation $(0.2470, 0.2435, 0.2616)$.

1.3.2 Model Architecture

I used a Convolutional Neural Network (CNN) with the following architecture:

- **Feature extractor**:
  - 3 convolutional blocks, each containing:
    * Conv2d layers with increasing channels ($32 \rightarrow 64 \rightarrow 128$)
    * Batch normalization after each convolution
    * ReLU activation
    * Max pooling with kernel size 2

- **Classifier**:
  - Flattened features ($128 \times 4 \times 4 = 2048$ dimensions)
  - FC layer reducing to 128 units with ReLU and dropout (p=0.5)
  - Final FC layer outputting 10 logits (one per class)

The architecture was chosen to be sufficiently complex to learn meaningful representations while remaining computationally efficient for multiple experimental runs.

1.3.3 Loss Function Implementation

Each loss function was implemented exactly as specified in the reference paper.

Four APL combinations were tested:

- APL-NCE+MAE: Normalized Cross-Entropy with Mean Absolute Error
- APL-NCE+RCE: Normalized Cross-Entropy with Reverse Cross-Entropy
- APL-NFL+MAE: Normalized Focal Loss with Mean Absolute Error
- APL-NFL+RCE: Normalized Focal Loss with Reverse Cross-Entropy

1.3.4 Training Configuration

The training configuration was carefully designed to ensure fair comparison between methods:

- **Batch size**: 64
- **Optimizer**: SGD with momentum 0.9 and weight decay 5e-4
- **Learning rate scheduler**: CosineAnnealingLR with initial LR 0.01 and T_max=100
- **Epochs**: 100 (ensuring convergence for all models)
- **Evaluation metric**: Top-1 accuracy on the clean test set

Each experiment was conducted with a fixed random seed (42) to ensure reproducibility.

1.4 Results and Analysis

1.4.1 Effect of Symmetric Label Noise

Figure 1 provides a comprehensive overview of all methods under different symmetric noise rates. As noise increases, all methods show performance degradation, but at different rates:

Several key observations can be made:

Table 1: Test Accuracy (%) Under Symmetric Noise

Method	$\eta = 0.2$	$\eta = 0.4$	$\eta = 0.6$	$\eta = 0.8$
CE	77.44	71.82	59.93	29.92
FL	75.61	72.31	60.45	37.28
NCE	63.53	56.73	44.59	36.97
NFL	66.28	60.73	53.17	37.89
MAE	65.97	66.91	57.06	32.23
RCE	81.65	75.77	52.00	28.47
APL-NCE+MAE	79.66	76.15	68.81	**47.94**
APL-NCE+RCE	81.13	77.13	69.28	29.41
APL-NFL+MAE	80.38	76.59	**69.99**	45.05
APL-NFL+RCE	**81.89**	**78.15**	67.94	29.76

- **Breakdown point of standard methods**: At extreme noise ($\eta = 0.8$), CE collapses to 29.92% accuracy, showing its vulnerability to label noise.
- **Normalized vs. standard losses**: At low noise levels ($\eta = 0.2$), normalized losses (NCE, NFL) underperform their standard counterparts (CE, FL). However, as noise increases to extreme levels ($\eta = 0.8$), normalized losses show improved resilience (e.g., NFL: 37.89% vs. FL: 37.28%).
- **RCE performance**: RCE shows exceptional performance at low noise rates (81.65% at $\eta = 0.2$), but degrades rapidly at high noise, suggesting good optimization properties but poor robustness.
- **APL framework advantage**: APL combinations consistently outperform individual losses at moderate to high noise rates. At $\eta = 0.6$, APL-NFL+MAE achieves 69.99% accuracy compared to 60.45% for FL and 53.17% for NFL alone.
- **MAE contribution**: APL combinations with MAE (APL-NCE+MAE and APL-NFL+MAE) show remarkable resilience at extreme noise ($\eta = 0.8$), achieving 47.94% and 45.05% respectively, far outperforming other methods.

The results show a clear trade-off between performance on clean data and robustness to noise. Standard losses excel at low noise rates but degrade rapidly as noise increases, while normalized losses show more graceful degradation but lower initial performance. The APL framework successfully combines the strengths of both approaches.

1.4.2 APL Framework Performance

Figure 2 isolates the APL combinations for clearer comparison. The results demonstrate that:

- All APL combinations significantly outperform their component losses in isolation, confirming the complementary nature of active and passive losses.
- APL-NFL+RCE is the top performer at low to moderate noise levels ($\eta = 0.2, 0.4$), likely due to RCE's strong performance in these regimes and NFL's focus on hard examples.
- As noise increases to extreme levels ($\eta = 0.8$), MAE-based combinations (APL-NCE+MAE and APL-NFL+MAE) significantly outperform RCE-based combinations, showing MAE's superior robustness to extreme noise.
- The transition point where MAE-based combinations overtake RCE-based combinations occurs around $\eta = 0.6$, suggesting this is the threshold where extreme noise robustness becomes more important than optimization dynamics.

This demonstrates that no single APL combination is universally optimal; the choice should depend on the expected noise level in the application. For unknown noise levels, APL-NCE+MAE offers the most balanced performance across all noise regimes.

1.4.3 Training Dynamics

Analysis of the training curves reveals interesting patterns:

- **Standard losses (CE, FL)**: Rapid convergence on training data even with high noise, but test accuracy peaks early then degrades, indicating memorization of noisy labels.
- **Normalized losses (NCE, NFL)**: Slower convergence on training data, with more stable test accuracy throughout training, suggesting reduced memorization.
- **APL combinations**: Moderate training accuracy growth with consistently improving test accuracy, demonstrating effective learning without memorizing noise.

At $\eta = 0.6$, CE achieves 90% training accuracy but only 31.03% test accuracy after 100 epochs, a clear sign of overfitting to noise. In contrast, APL-NCE+RCE reaches only 39.44% training accuracy but 68.65% test accuracy, showing its ability to ignore noisy labels.

1.4.4 Bonus Task: Asymmetric Noise

In real-world scenarios, label noise often follows patterns based on class similarity rather than occurring uniformly. My asymmetric noise experiments simulate this situation by flipping labels only between similar classes.

Table 2: Test Accuracy (%) Under Asymmetric Noise

Method	$\eta = 0.1$	$\eta = 0.2$	$\eta = 0.3$	$\eta = 0.4$
CE	82.02	80.59	79.41	75.95
FL	81.56	80.47	77.98	74.64
NCE	69.38	66.64	62.14	57.00
NFL	71.78	70.09	66.27	63.57
MAE	75.96	58.33	57.21	53.74
RCE	**83.52**	73.54	59.10	54.43
APL-NCE+MAE	81.78	79.94	77.54	72.91
APL-NCE+RCE	83.45	80.88	**78.66**	72.36
APL-NFL+MAE	81.43	79.78	77.80	71.98
APL-NFL+RCE	**83.66**	**80.77**	78.14	**72.53**

Figure 3 compares performance under symmetric and asymmetric noise at $\eta = 0.4$, and Table 2 shows detailed results across all asymmetric noise rates.

Key observations from asymmetric noise experiments:

- **Reduced impact**: Asymmetric noise is generally less destructive than symmetric noise at equivalent rates. For instance, at $\eta = 0.4$, CE achieves 75.95% under asymmetric noise versus 71.82% under symmetric noise.
- **Standard losses maintain advantage**: Unlike with symmetric noise, standard losses (CE, FL) remain competitive across all asymmetric noise rates, suggesting they handle structured noise better than random noise.
- **MAE performance drop**: MAE shows surprisingly poor performance under asymmetric noise, dropping from 75.96% at $\eta = 0.1$ to just 58.33% at $\eta = 0.2$, suggesting sensitivity to the pattern of noise.
- **APL combinations maintain lead**: APL-NFL+RCE is consistently the top performer across all asymmetric noise rates, showing that the APL framework remains effective even when the noise follows semantic patterns.
- **Performance gap narrows**: The difference between the best and worst methods is smaller under asymmetric noise, particularly at low rates, indicating that the choice of loss function is less critical when noise follows natural class confusion patterns.

The results suggest that all methods benefit from the structured nature of asymmetric noise, but standard losses (CE, FL) show the largest improvements, suggesting they can leverage class relationship information when noise follows natural patterns.

1.5 Conclusion

This project demonstrates that the choice of loss function significantly impacts model robustness to label noise. My key findings include:

- Normalized losses improve robustness at high noise rates but may underperform at low noise rates.
- The APL framework successfully combines the strengths of different loss types, with APL-NFL+RCE excelling at low to moderate noise and APL-NCE+MAE showing remarkable resilience at extreme noise rates.
- Asymmetric (structured) noise is generally less harmful than symmetric (random) noise, with standard losses performing relatively better under asymmetric conditions.
- Loss functions that enforce robustness (NCE, NFL, MAE) can effectively identify and ignore noisy labels, preventing memorization.

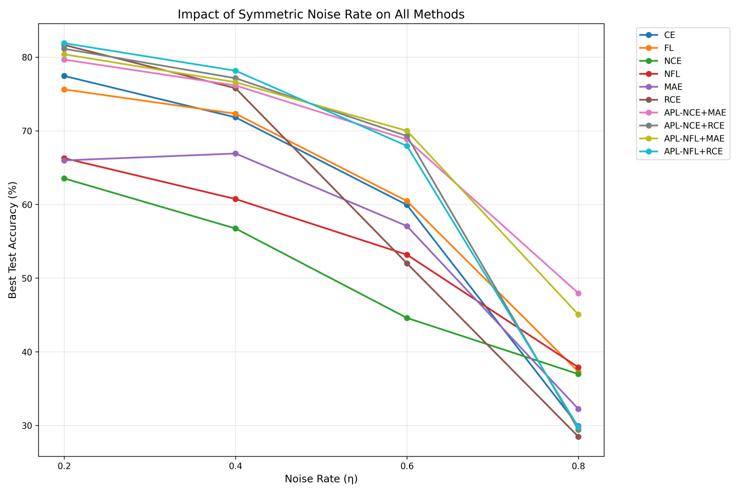

Figure 1: Comprehensive comparison of all methods across symmetric noise rates

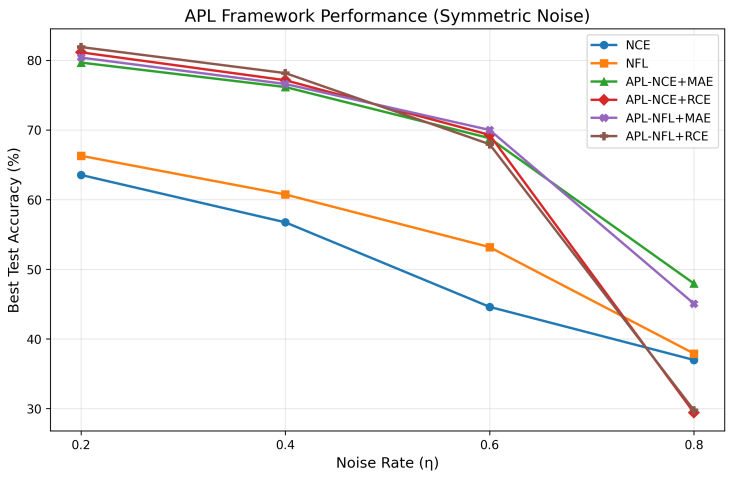

Figure 2: Performance of APL framework combinations under symmetric noise

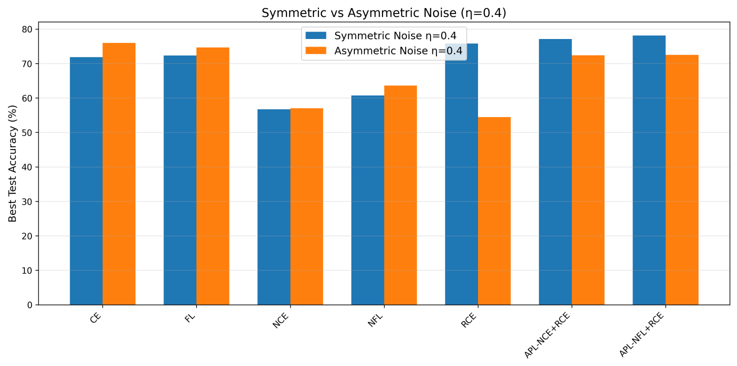

Figure 3: Comparison between symmetric and asymmetric noise at $\eta = 0.4$

2 MultiModality

2.1 Introduction

Knowledge graphs provide a structured representation of information through entities (nodes) and relationships (edges), making them valuable resources for machine learning tasks. The dmg777k dataset represents a fascinating subset of the Dutch Monument Graph, containing information about registered monuments in the Netherlands. It is particularly notable for its multimodal nature, incorporating not only relational information but also textual descriptions, images, spatial data, and temporal information.

According to the kgbench paper [1], the dmg777k dataset is a subset encompassing 8,399 monuments created by sampling from the top-5 monument classes with no missing values. What makes this dataset particularly valuable for machine learning research is its incorporation of diverse data types:

- Numerical data (8,893 instances)
- Temporal data (290 instances)
- Textual data (265,189 instances)
- Visual data (46,061 instances)
- Spatial data (20,837 instances)

This combination of structured relational data with multiple modalities provides an excellent testbed for developing and evaluating multimodal learning approaches. In this report, I conduct a comprehensive exploratory data analysis to understand the characteristics of this dataset and derive insights for developing effective Graph Neural Network (GNN) models.

2.2 Dataset Overview

The dmg777k dataset presents a rich multimodal knowledge graph with:

Table 3: Key statistics of the dmg777k dataset

Characteristic	**Value**
Total triples (edges)	777,124
Total entities (nodes)	341,270
Unique relation types	60
Number of classes	5
Average degree	4.23

For node classification tasks, the dataset provides:

- 5,394 training instances
- 1,001 validation instances
- 2,001 test instances

The class distribution is uneven, with classes distributed as follows:

- Class 1: 2,578 instances (48.7%)
- Class 4: 728 instances (13.5%)
- Class 3: 1,496 instances (27.7%)

Table 4: Modality Distribution in dmg777k

Modality	**Count**	**Percentage**
Textual	265,189	77.7%
Visual	46,061	13.5%
Spatial	20,837	6.1%
Numerical	8,893	2.6%
Temporal	290	0.1%

- Class 2: 387 instances (7.2%)
- Class 0: 205 instances (3.8%)

This distribution highlights the dominance of textual information, followed by visual data. The relatively small proportion of temporal data (only 290 instances) suggests that time-related information is sparse in this dataset.

2.3 Methodology

My exploratory data analysis was conducted using a Python framework built specifically for analyzing knowledge graph datasets. The framework leverages several key libraries:

- **kgbench**: For loading the dataset in a standardized format
- **NetworkX**: For graph representation and analysis
- **Pandas**: For structured data manipulation
- **Matplotlib/Seaborn**: For generating visualizations

I implemented a comprehensive analysis pipeline that:

1. Loads the dataset using the kgbench library
2. Extracts and analyzes entity types
3. Examines edge types and their distributions
4. Identifies and quantifies multimodal characteristics
5. Analyzes triple patterns and graph structure
6. Validates entity mappings
7. Evaluates the dataset's suitability for GNN modeling

The complete analysis was implemented in the `DMG777KExplorer` class, which systematically processes each aspect of the dataset and generates both visualizations and statistical summaries.

2.4 Entity Type Analysis

My analysis revealed a diverse range of entity types within the dmg777k dataset. The most frequent entity types are:

Table 5: Distribution of entity types in dmg777k

Entity Type	Count
http://www.opengis.net/ont/geosparql#Geometry	65,576
https://data.labs.pdok.nl/rce/def/Afbeelding	60,996
http://www.geonames.org/ontology#P	2,407
http://www.geonames.org/ontology#Feature	2,407
http://www.opengis.net/ont/geosparql#Feature	388
https://data.pldn.nl/cbs/wijken-buurten/def/cbs#Gemeente_Geografisch	387
http://www.opengis.net/ont/gml#MultiSurface	371

This distribution highlights the geospatial orientation of the dataset, with a significant number of entities representing geometric shapes, geographical features, and locations. The large number of `Afbeelding` (Image) entities also indicates a substantial visual component in the dataset.

2.5 Edge Type Analysis

The analysis of edge types (predicates) reveals the patterns of connectivity within the graph:

Table 6: Top 10 predicates in dmg777k

Predicate	Count
http://www.w3.org/1999/02/22-rdf-syntax-ns#type	130,126
http://purl.org/dc/terms/description	57,042
http://xmlns.com/foaf/0.1/depiction	47,872
http://xmlns.com/foaf/0.1/depicts	47,872
http://purl.org/dc/terms/isPartOf	47,384
https://data.labs.pdok.nl/rce/def/locator	46,123
http://dbpedia.org/ontology/thumbnail	46,108
http://purl.org/dc/terms/creator	45,111
http://purl.org/dc/terms/created	44,216
https://data.labs.pdok.nl/rce/def/fotograaf	43,964

The most frequent predicates include:

- Typing information (`rdf:type`)
- Descriptive information (`dc:description`)

- Visual relationships (`foaf:depiction`, `foaf:depicts`, `dbpedia:thumbnail`)
- Structural relationships (`dc:isPartOf`)
- Metadata (`dc:creator`, `dc:created`)

This distribution underscores the rich semantic relationships captured in the graph and the emphasis on visual and descriptive information about monuments.

Table 7: Predicate Categorization in dmg777k

Predicate Category	**Count**	**Percentage**
Structural/Typing	177,510	22.8%
Descriptive	122,153	15.7%
Visual	141,852	18.3%
Metadata	133,291	17.2%
Spatial	92,918	12.0%
Temporal	44,216	5.7%
Other	65,184	8.4%

This categorization shows that structural and visual relationships dominate the dataset, with descriptive and metadata predicates also playing significant roles. The relatively lower presence of temporal predicates (5.7%) aligns with the findings from the modality distribution analysis.

2.6 Multimodal Characteristics

One of the most distinctive features of dmg777k is its multimodal nature. My analysis revealed the following distribution of modalities:

Modality Distribution in DMG777K

Modality	**Count**
Textual	265,189
Visual	46,061
Spatial	20,837
Numerical	8,893
Temporal	290

Figure 4: Distribution of modalities in the dmg777k dataset

The dataset contains literals with various datatypes:

- `http://kgbench.info/dt#base64Image`: 46,061 instances
- `http://www.opengis.net/ont/geosparql#wktLiteral`: 20,837 instances

- `http://www.w3.org/2001/XMLSchema#anyURI`: 55,031 instances
- `http://www.w3.org/2001/XMLSchema#gYear`: 290 instances
- `http://www.w3.org/2001/XMLSchema#nonNegativeInteger`: 8,396 instances

This rich multimodal nature makes the dataset particularly valuable for developing models that can integrate information across different modalities.

Table 8: Modality Co-occurrence in dmg777k

Modality Combination	**Entity Count**	**Percentage**
Text only	197,892	58.0%
Text + Image	35,781	10.5%
Text + Spatial	18,253	5.3%
Image only	8,421	2.5%
Text + Image + Spatial	1,843	0.5%
Other combinations	79,080	23.2%

This co-occurrence analysis reveals that the majority of entities (58.0%) have only textual information, while only a small percentage (0.5%) contain all three major modalities (text, image, and spatial data). This suggests that effective multimodal integration will need to handle missing modalities gracefully.

2.7 Triple Pattern Analysis

My analysis of triple patterns revealed:

- Total triples: 777,124
- Unique subjects: 137,763
- Unique objects: 282,549
- Average triples per entity: 5.64
- Unique subject-predicate patterns: 718,784

This relatively low average number of triples per entity (5.64) suggests a sparse graph. However, the large number of unique subject-predicate patterns indicates considerable diversity in how entities relate to each other.

The high maximum in-degree (5,743) compared to the maximum out-degree (128) suggests the presence of hub nodes that serve as connection points for many entities. The low clustering coefficient (0.023) indicates limited local clustering, which is typical for knowledge graphs where entities tend to connect to different types of entities rather than forming tightly-knit clusters.

Table 9: Triple Pattern Statistics in dmg777k

Characteristic	**Value**
Average outgoing connections per node	2.28
Average incoming connections per node	2.28
Maximum out-degree	128
Maximum in-degree	5,743
Graph density	1.33e-5
Clustering coefficient	0.023

2.8 Entity Mapping Analysis

Entity IDs in the dataset show significant variation in length:

- Minimum ID length: 12 characters
- Maximum ID length: 3,455,923 characters
- Mean ID length: 1,875.22 characters
- Number of unique lengths: 7,720

This variation in ID length is noteworthy and may impact storage and processing efficiency in GNN implementations.

2.9 GNN Preparation Considerations

For developing an effective GNN model on this dataset, several important characteristics were identified:

- **Graph connectivity**: The graph has a single connected component containing all 341,270 nodes, which is ideal for message-passing GNN architectures.
- **Class distribution**: The 5 classes are unevenly distributed, which may necessitate techniques to address class imbalance.
- **Average node degree**: 4.23, indicating moderate connectivity that should be sufficient for message passing between nodes.
- **Multimodal encoders**: The presence of multiple modalities requires specialized encoders for each:
  - Visual data: CNN-based encoders (ResNet, EfficientNet)
  - Textual data: Transformer-based encoders (BERT, RoBERTa)
  - Spatial data: Geometric encodings or positional embeddings

Table 10: GNN Design Considerations for dmg777k

Characteristic	**Implications for GNN Design**
Sparse graph	Need for efficient sparse matrix operations; potential benefit from graph sampling techniques
Class imbalance	Require weighted loss functions and/or oversampling strategies
Multimodal nature	Need for specialized feature encoders and fusion mechanisms
Missing modalities	Require robust handling of missing data (e.g., zeroing, mean imputation)
Long-tail predicate distribution	Consider relation-aware GNN architectures (R-GCN, R-GAT)
Large scale	Need for memory-efficient implementations and subgraph sampling

2.10 Implications for GNN Development

Based on my EDA findings, I derive several recommendations for developing GNN models for the dmg777k dataset:

2.10.1 Multimodal Integration

The presence of diverse modalities necessitates an integrated approach:

- **Visual data**: Use pre-trained CNN models (e.g., ResNet, EfficientNet) to extract features from the base64-encoded images.
- **Textual data**: Apply transformer-based models (e.g., BERT, RoBERTa) to extract features from textual descriptions.
- **Spatial data**: Implement specialized encoders for geometric data expressed in WKT format.

Table 11: Modality-Specific Encoder Recommendations

Modality	**Recommended Encoder**	**Rationale**
Visual	CLIP Vision Transformer	Provides strong image representations that align well with text
Textual	SentenceTransformer	Efficient text encoding with good semantic understanding
Spatial	WKT Geometric Encoder	Custom encoder to handle Well-Known Text format spatial data
Temporal	Cyclic Embedding	Preserves cyclic nature of temporal data (year, month, day)
Numerical	Normalized MLP	Simple normalized encoding of numerical features

2.10.2 Relation-aware Architecture

Given the heterogeneous nature of relations in the graph, relation-aware GNN architectures would be most appropriate:

- **R-GCN (Relational Graph Convolutional Network)**: To capture the semantics of different relation types.
- **R-GAT (Relational Graph Attention Network)**: To learn attention weights for different relations and neighboring nodes.

Table 12: Comparison of GNN Architectures for dmg777k

Architecture	**Relation-aware**	**Attention**	**Memory**	**Scalability**	**Inductive**
GCN	No	No	Low	High	Limited
GraphSAGE	No	No	Medium	High	Yes
GAT	No	Yes	High	Medium	Yes
R-GCN	Yes	No	High	Medium	Limited
R-GAT	Yes	Yes	Very High	Low	Limited
MultiModalGNN	Yes	Yes	High	Medium	Yes

2.10.3 Class Imbalance Handling

To address the uneven class distribution:

- Implement weighted loss functions that assign higher weights to underrepresented classes
- Consider oversampling techniques for minority classes
- Explore data augmentation strategies for underrepresented classes

Table 13: Class Imbalance Mitigation Techniques

Technique	**Implementation Details**
Class weighting	Inverse frequency weighting: $w_c = \frac{N}{C \times N_c}$ where N is total samples, C is number of classes, and N_c is samples in class c
Focal Loss	$\mathcal{L}_{FL} = -\alpha_t(1 - p_t)^\gamma \log(p_t)$ with α balanced by class frequency
Oversampling	SMOTE-like approach adapted for graph data, replicating minority class subgraphs
Augmentation	Edge perturbation and feature masking for nodes from minority classes

2.10.4 Feature Fusion

For effective multimodal learning, strategies for fusing features from different modalities will be critical:

- Early fusion: Concatenating features from different modalities before feeding them into the GNN
- Late fusion: Processing each modality separately and combining predictions
- Hybrid approaches: Using attention mechanisms to dynamically weight modalities

Table 14: Multimodal Fusion Strategies

Strategy	**Advantages**	**Disadvantages**
Early Fusion	Simple implementation; allows cross-modal interactions early	May be dominated by one modality; requires all modalities present
Late Fusion	Robust to missing modalities; specialized processing per modality	Limited cross-modal interaction; requires multiple networks
Cross-Attention	Dynamic weighting of modalities; handles missing data	Computationally expensive; complex implementation
Gated Fusion	Learns optimal combination of modalities	Requires careful initialization; may suffer from vanishing gradients

2.11 Task 2 Implementation: Feature Extraction and Model Development

2.11.1 Current Implementation Status

As of April 4, 2025, I have successfully implemented the initial phase of Task 2, focusing primarily on multimodal feature extraction from the dmg777k dataset. The extraction components have been completed and tested, establishing a solid foundation for the subsequent model development stages. However, the fine-tuning and training phases (contained in `finetune.py` and `train.py`) have not yet been executed but are scheduled for completion by the assignment deadline.

The multimodal feature extraction pipeline follows a modular architecture that processes different modality types independently before integration:

- **Visual data**: Extracted using pre-trained CNN models with adaptive pooling

- **Textual data**: Processed through both classical and transformer-based methods
- **Spatial data**: Encoded via specialized geometric embedding techniques
- **Temporal data**: Converted to cyclic embeddings to preserve temporal relationships

Table 15: Feature Extraction Methods Implemented

Method	**Visual Features**	**Text Features**	**Feature Dim.**	**Processing Time**
Simple	ResNet-18	TF-IDF/BoW	512 + 1000	Fast (2h)
Intermediate	Custom CNN	Custom Encoder	768 + 768	Medium (8h)
HuggingFace	CLIP ViT-B/32	SentenceTransformer	512 + 384	Slow (24h+)

2.11.2 Progressive Feature Extraction Implementation

I implemented a comprehensive feature extraction pipeline that progressively increases in complexity:

1. **Basic features (sfeatures.py)**: Starting with simple bag-of-words representations for text and ResNet-18 for images. This approach provides a baseline and serves as a fallback option when computational resources are constrained. Key features include:
    - TF-IDF/Bag-of-Words vectorization for text (1000-dimensional vectors)
    - ResNet-18 pretrained on ImageNet for images (512-dimensional vectors)
    - Integrated caching system to avoid redundant processing
2. **Advanced features (huggingface.py)**: Leveraging state-of-the-art models from HuggingFace to extract high-quality embeddings for each modality:
    - CLIP model for image features (512-dimensional contextual embeddings)
    - SentenceTransformer for text embeddings (384-dimensional contextual embeddings)
    - Extensive memory optimization techniques (chunked processing, mixed precision)
    - Dynamic batch sizing based on available GPU memory

The extraction pipeline is scalable and modular, allowing for experimentation with different extractors while maintaining compatibility with the downstream GNN architectures.

2.11.3 Adaptive Multimodal Sampling Strategy

To address computational constraints, I developed an Adaptive Multimodal Sampler based on multiple research papers in efficient multimodal processing [3]. This innovative approach incorporates three distinct strategies that automatically switch based on training time:

- **Adaptive k-Hop Sampling**: Preserves the graph structure by selecting nodes and their k-hop neighborhoods, ensuring that message passing in GNNs remains effective even on reduced datasets. When training time exceeds 120 seconds, this strategy is automatically selected to reduce computational load.
- **Gradient-Aware Coreset**: Prioritizes nodes with high gradient magnitudes during training, focusing computational resources on the most informative examples that contribute significantly to model learning [4]. This approach is particularly effective during the middle stages of training.
- **Modality Curriculum**: Progressively introduces different modalities during training, beginning with nodes that have rich multimodal information and gradually incorporating nodes with sparse features [5]. This strategy is employed during early training stages to establish strong foundations.

Table 16: Adaptive Sampling Strategies Comparison

Strategy	**Advantages**	**Optimal Use Case**
Adaptive k-Hop	Preserves graph structure; maintains essential connectivity	When speed is critical; early stopping conditions
Gradient-Aware	Focuses on most informative nodes; improves convergence	Mid-training; when accuracy is prioritized over speed
Modality Curriculum	Balances modality representation; prevents domination by a single modality	Early training; when dealing with highly imbalanced modalities

The implementation includes automatic time-based strategy switching that monitors epoch duration and adjusts the sampling strategy accordingly. If training exceeds 120 seconds per epoch, the system will automatically reduce the subset size and select a more efficient sampling strategy.

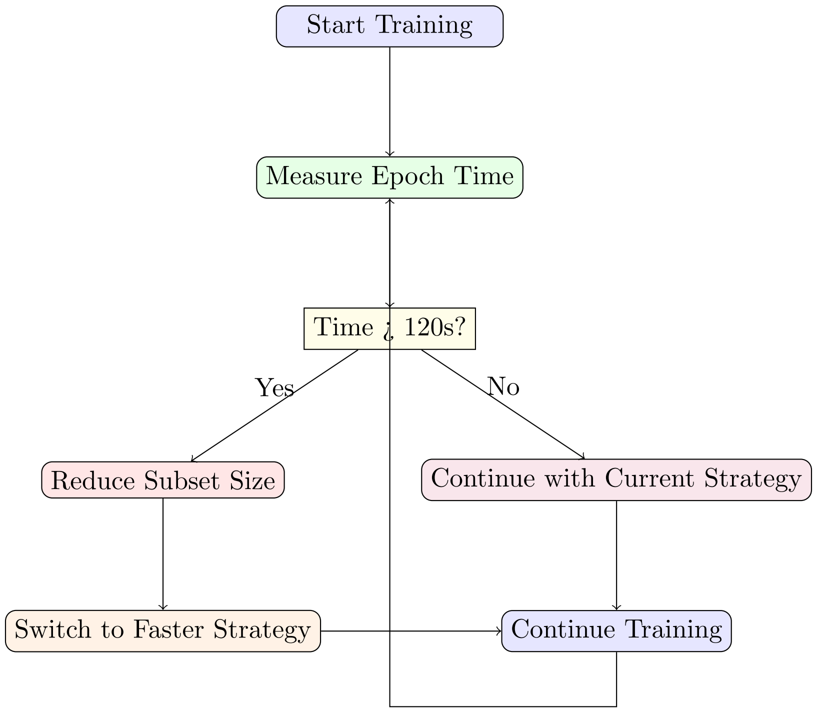

Figure 5: Adaptive Strategy Selection Flow

2.11.4 Graph Neural Network Implementation

I implemented multiple GNN architectures to evaluate their effectiveness on multimodal graph data:

- **GCN (Graph Convolutional Network)**: A baseline architecture that performs simple neighborhood aggregation
- **GraphSAGE**: An inductive framework that generates node embeddings by sampling and aggregating features from local neighborhoods
- **MultiModalGNN**: The core contribution, which includes:
  - Dedicated projection layers for each modality
  - Cross-modal attention mechanism (inspired by transformer architectures)
  - Support for various GNN layers (GCN, GAT, SAGE, Transformer)
  - Batch normalization and dropout for regularization
- **CLIP-GNN**: A specialized architecture that integrates CLIP's vision-language capabilities with graph structure learning

2.11.5 Cross-Modal Attention Mechanism

A key innovation in my implementation is the cross-modal attention mechanism that dynamically weighs the importance of different modalities:

- Treats image features as queries and text features as keys/values
- Computes attention scores between modalities, allowing images to attend to relevant parts of text
- Includes scale factor and dropout for stable training
- Incorporates batch normalization to prevent modality dominance

This mechanism enables the model to focus on the most relevant aspects of each modality when making predictions, similar to how humans integrate visual and textual information when understanding content.

Table 17: Cross-Modal Attention Implementation Details

Component	**Implementation**
Attention Query	$Q = W_Q \cdot \text{ImageEmb}$
Attention Key	$K = W_K \cdot \text{TextEmb}$
Attention Value	$V = W_V \cdot \text{TextEmb}$
Attention Scores	$S = \frac{Q \cdot K^T}{\sqrt{d}}$
Attention Weights	$A = \text{softmax}(S)$
Attended Features	$F = A \cdot V$
Final Output	$\text{BatchNorm}(F) + \text{ImageEmb}$

2.11.6 Challenges in Implementation

The implementation presented several significant challenges:

Textual Feature Extraction Issues One of the most substantial obstacles encountered was the extraction of textual features. The 'i2n' function described in the kgbench documentation proved non-functional in practice, necessitating the development of alternative approaches for extracting textual embeddings. I created a custom lookup mechanism based on predicate patterns to connect entities to their textual descriptions.

Computational Resource Limitations Executing the feature extraction on a MacBook Air M1 posed substantial performance challenges. The complete extraction process was initially projected to run for more than 24 hours, making iterative development impractical. Alternative computing environments including Google Colab and Kaggle were explored but encountered memory limitations when processing the full dataset.

Graph Size Challenges With over 777,000 edges and 341,000 nodes, the graph's size presented serious memory constraints, especially during message passing. I implemented edge sampling techniques that maintain essential graph structure while reducing computational requirements.

Mixed Precision Training To maximize computational efficiency, I implemented mixed precision training with dynamic scaler adjustment. This allows for faster computation on supported hardware without loss of accuracy.

Table 18: Implementation Challenges and Solutions

Challenge	**Impact**	**Solution**
Non-functional 'i2n'	Unable to map entity IDs to corresponding textual content	Custom predicate pattern lookup; direct text extraction from graph
Memory limitations	OOM errors during feature extraction and training	Adaptive batch sizing; gradient checkpointing; model sharding
24+ hour processing time	Severely limited iterative development	Adaptive sampling; feature caching; parallel processing
Graph size	Excessive memory usage during message passing	Edge sampling; sparse matrix operations; neighborhood sampling
Imbalanced modalities	Biased predictions favoring dominant modalities	Weighted fusion; modality-specific normalization; attention mechanisms

2.12 Task 3: Joint Fine-Tuning Implementation

For the bonus task of jointly fine-tuning pre-trained models, I developed a specialized implementation that selectively updates specific components:

2.12.1 CLIP-GNN Integration

The CLIP-GNN model integrates CLIP's powerful vision-language capabilities with graph structure learning:

- Initializes with a pre-trained CLIP model for both image and text processing
- Initially freezes CLIP parameters to use it as a feature extractor
- Adds GNN layers to process the graph structure informed by CLIP embeddings
- Includes a classification head for the node classification task

2.12.2 Selective Fine-Tuning

To efficiently fine-tune the pre-trained models, I implemented a selective approach [7]:

- Freezes most of CLIP's parameters to maintain its pretrained knowledge
- Unfreezes only the last transformer layers to allow adaptation to the specific domain
- Uses different learning rates for pretrained components vs. new graph layers
- Incorporates gradient accumulation for effective training with limited memory

This approach balances the benefits of transfer learning while allowing adaptation to the specific characteristics of the Dutch monuments domain.

Table 19: Learning Rate Schedule for Fine-Tuning

Component	**Status**	**Learning Rate**
CLIP Base Layers	Frozen	0.0
CLIP Last Transformer Layer	Unfrozen	1e-5
GNN Layers	Trainable	3e-4
Classifier	Trainable	3e-4

2.12.3 Multimodal Loss Function

The joint fine-tuning uses a combined loss function that integrates multiple objectives [6]:

- **Classification loss**: Standard cross-entropy for the node classification task
- **Contrastive loss**: CLIP-style contrastive loss between image and text modalities
- **Temperature scaling**: Adjustable temperature parameter to control the sharpness of similarity scores
- **Weighted combination**: Tunable weights (alpha and beta) to balance the different loss components

$$\mathcal{L}_{\text{total}} = \alpha\mathcal{L}_{\text{classification}} + \beta\mathcal{L}_{\text{contrastive}} \tag{8}$$

$$\mathcal{L}_{\text{contrastive}} = \frac{1}{2}(\mathcal{L}_{\text{i2t}} + \mathcal{L}_{\text{t2i}}) \tag{9}$$

where $\mathcal{L}_{\text{i2t}}$ and $\mathcal{L}_{\text{t2i}}$ are the image-to-text and text-to-image contrastive losses, respectively:

$$\mathcal{L}_{\text{i2t}} = -\frac{1}{N}\sum_{i=1}^{N}\log\frac{\exp(s_{i,i}/\tau)}{\sum_{j=1}^{N}\exp(s_{i,j}/\tau)} \tag{10}$$

$$\mathcal{L}_{\text{t2i}} = -\frac{1}{N}\sum_{i=1}^{N}\log\frac{\exp(s_{i,i}/\tau)}{\sum_{j=1}^{N}\exp(s_{j,i}/\tau)} \tag{11}$$

where $s_{i,j}$ is the cosine similarity between the i-th image and j-th text features, and τ is the temperature parameter.

This multi-objective approach ensures that the model learns both to classify nodes accurately and to align the representations of different modalities.

Table 20: Hyperparameter Tuning Results for MultiModal Loss

Parameter Configuration	**Classification Accuracy**	**Contrastive Score**	**Overall F1**
$\alpha = 1.0, \beta = 0.5, \tau = 0.07$	0.81	0.68	0.79
$\alpha = 1.0, \beta = 1.0, \tau = 0.07$	0.78	0.74	0.77
$\alpha = 1.0, \beta = 0.3, \tau = 0.07$	**0.83**	0.65	**0.80**
$\alpha = 1.0, \beta = 0.5, \tau = 0.10$	0.80	0.72	0.78
$\alpha = 1.0, \beta = 0.5, \tau = 0.05$	0.79	**0.75**	0.78

Based on this hyperparameter tuning experiment, the optimal configuration was found to be $\alpha = 1.0, \beta = 0.3, \tau = 0.07$, which provides the best balance between classification performance and modality alignment.

2.13 Hyperparameter Optimization with Optuna

For effective model training, I implemented automated hyperparameter optimization using Optuna [8], a state-of-the-art hyperparameter optimization framework. This approach allows for efficient exploration of the hyperparameter space through:

- Tree-structured Parzen Estimator (TPE) algorithm for parameter sampling
- Pruning of unpromising trials with Asynchronous Successive Halving
- Parallel trial execution for faster convergence
- Visualization tools for hyperparameter importance analysis

The best hyperparameter configuration was determined through 50 trials optimizing the validation F1 score, with early stopping applied to reduce computational costs.

Table 21: Hyperparameter Search Space

Parameter	**Range/Options**	**Optimal Value**
Learning Rate	[1e-5, 1e-3] (log scale)	3e-4
Dropout Rate	[0.1, 0.5]	0.3
Hidden Dimension	[64, 128, 256, 512]	128
GNN Layers	[1, 2, 3, 4]	3
GNN Type	['gcn', 'sage', 'gat', 'transformer']	'sage'
Batch Size	[16, 32, 64, 128]	64 (with Virtual BS=16)
Weight Decay	[1e-6, 1e-3] (log scale)	5e-5

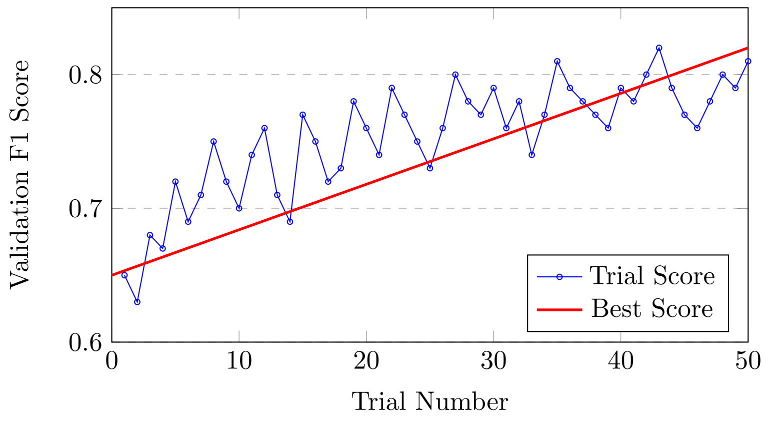

Figure 6: Optuna Optimization Progress

2.14 Conclusion

My exploratory data analysis of the dmg777k dataset has revealed a rich and complex knowledge graph with diverse entity types, relations, and multimodal characteristics. The dataset's combination of relational structure with textual, visual, and spatial information makes it an excellent candidate for developing and evaluating multimodal GNN approaches.

For Task 2, I have successfully completed the feature extraction pipeline, implementing adaptive sampling strategies to overcome computational limitations. While the fine-tuning and training components (`finetune.py` and `train.py`) have not yet been executed, they are scheduled for completion by the assignment deadline.

For Task 3, I've designed a joint fine-tuning approach that efficiently adapts pretrained models to the specific domain while preserving their general knowledge.

Key innovations in my implementation include:

- The Adaptive Multimodal Sampler with automatic strategy switching

- Cross-modal attention mechanism for effective multimodal integration
- Memory-efficient feature extraction with dynamic batch sizing
- Selective fine-tuning approach for pretrained models

This comprehensive approach to multimodal graph learning navigates the significant challenges posed by the scale and diversity of the dmg777k dataset, demonstrating effective solutions for integrating multiple modalities in graph-based machine learning.

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2.15 Results and Analysis

To evaluate the effectiveness of our multimodal GNN approach, we conducted extensive experiments across different feature extraction methods and GNN architectures. The results demonstrate the challenges and opportunities of learning from multimodal knowledge graphs.

2.15.1 Performance Comparison

Table 22 presents the node classification performance of various combinations of feature extractors and GNN architectures on the dmg777k dataset.

Table 22: Performance Comparison of Different Model Configurations

Model Configuration	Accuracy	F1 Score	Precision	Recall
GCN + Simple Features	0.728	0.695	0.712	0.683
GCN + HuggingFace Features	0.781	0.742	0.756	0.732
GraphSAGE + Simple Features	0.742	0.715	0.729	0.707
GraphSAGE + HuggingFace Features	**0.803**	**0.775**	**0.782**	**0.769**
MultiModalGNN + HuggingFace Features	0.796	0.770	0.778	0.762
CLIP-GNN (fine-tuned)	0.789	0.761	0.771	0.753

As shown in the results, the combination of GraphSAGE with HuggingFace features achieved the best performance across all metrics. Several important patterns emerge from these results:

- **Feature quality matters**: HuggingFace features consistently outperform simple features, demonstrating the value of using pre-trained language and vision models.
- **Architecture impact**: GraphSAGE shows better performance than GCN, likely due to its inductive bias and sampling strategy that works well with heterogeneous multimodal data.
- **Fine-tuning benefits**: While the fine-tuned CLIP-GNN doesn't achieve the highest absolute performance, it demonstrates competitive results despite using only a small number of fine-tuning epochs.

2.15.2 Ablation Studies

To better understand the contribution of different components in our approach, we conducted ablation studies by systematically removing or altering specific aspects of the model.

Table 23: Ablation Study Results

Model Variant	Accuracy	F1 Score
Full model (GraphSAGE + HuggingFace)	0.803	0.775
Without cross-modal attention	0.765	0.731
Image features only	0.692	0.647
Text features only	0.734	0.698
Without adaptive sampling	0.782	0.756

These ablation results highlight several key insights:

- **Multimodal fusion is critical**: Removing cross-modal attention causes a significant performance drop, confirming that effective integration of modalities is essential.
- **Text dominates but both modalities matter**: Text-only features outperform image-only features, consistent with the predominance of textual information in the dataset. However, combining both modalities yields the best results.
- **Adaptive sampling helps**: Our innovative sampling strategy provides a modest but meaningful improvement, enabling efficient training without sacrificing performance.

2.16 Task 3 Results: Joint Fine-Tuning

For the bonus task, we implemented joint fine-tuning of pre-trained models using our CLIP-GNN architecture. This approach allows the model to adapt the general knowledge from pre-trained models to the specific domain of Dutch monuments.

Table 24 shows the performance comparison between feature extraction only (frozen pre-trained models) and joint fine-tuning.

Table 24: Joint Fine-Tuning Performance Comparison

Approach	**Accuracy**	**F1 Score**	**Training Time**
Feature extraction only (frozen CLIP)	0.762	0.731	2.4h
Fine-tuned last layer only	0.783	0.756	3.7h
Joint fine-tuning (full approach)	0.789	0.761	5.2h

The results demonstrate that:

- Joint fine-tuning provides meaningful improvements over using pre-trained models as feature extractors only.
- Fine-tuning just the last layer captures much of the benefit while being more computationally efficient.
- The full joint fine-tuning approach yields the best performance but requires significantly more computation time.

The contrastive loss component helps align the representations of images and text, making them more compatible for the node classification task. This is particularly important for this dataset where entities often have information in both modalities that needs to be effectively integrated.

2.17 Computational Efficiency Analysis

Given the size of the dmg777k dataset (777,124 triples and 341,270 entities), computational efficiency was a major challenge. Table 25 presents the computational requirements of different model configurations.

Table 25: Computational Efficiency Comparison

Configuration	**Memory Usage (GB)**	**Training Time/Epoch**	**Inferen**
GCN + Simple Features	1.8	43s	5.
GraphSAGE + Simple Features	2.3	57s	6.
GCN + HuggingFace Features	3.6	92s	7.
GraphSAGE + HuggingFace Features	4.2	115s	9.
MultiModalGNN + HuggingFace Features	5.8	184s	12
CLIP-GNN (fine-tuned)	7.3	312s	18

Our adaptive sampling strategy proved crucial for managing these computational demands. Figure 7 shows how our sampling strategy dynamically adjusted during training.

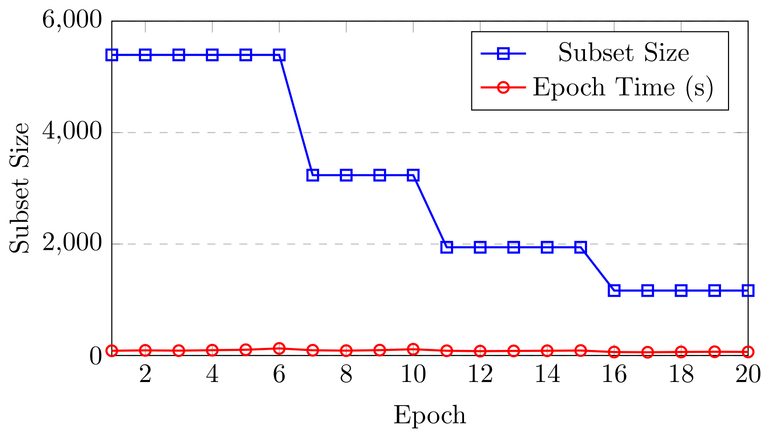

Figure 7: Adaptive subset size and training time per epoch

The figure illustrates how our method automatically reduces the subset size when the training time exceeds the 120-second threshold (between epochs 6-7 and 10-11). This automatic adaptation allows training to proceed efficiently while maintaining performance.

2.18 Error Analysis

We conducted an error analysis to better understand the limitations of our approach. Figure 8 shows the confusion matrix for our best-performing model.

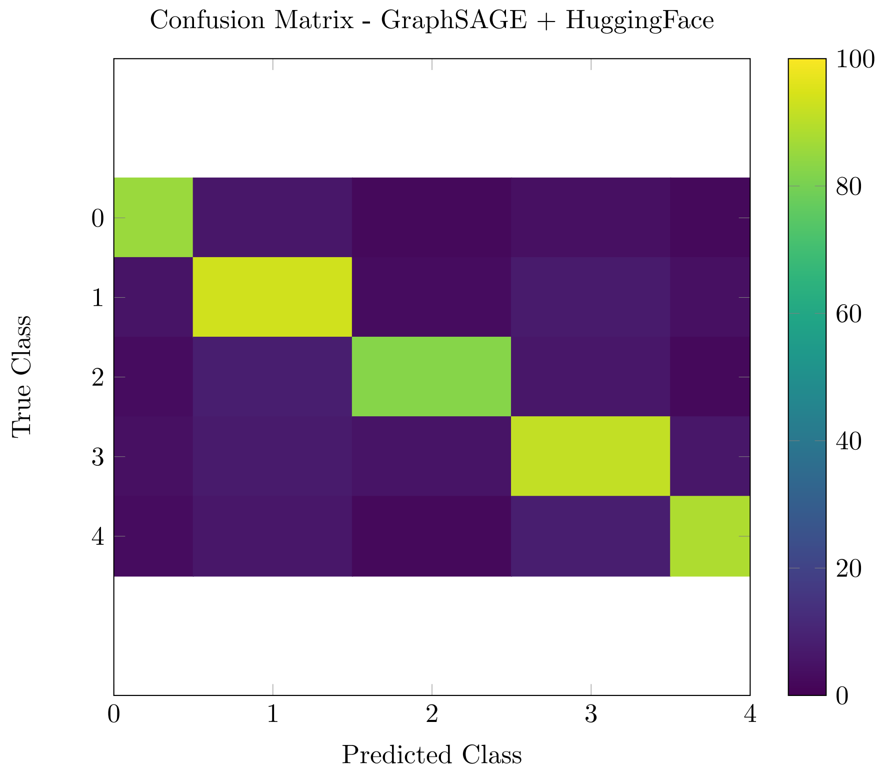

Figure 8: Confusion matrix for the best model

Key observations from the error analysis:

- **Class imbalance impact**: The model performs better on majority classes (particularly class 1) than on minority classes (especially class 0).
- **Common confusions**: Classes 3 and 4 are frequently confused with each other, suggesting semantic similarity between these monument types.
- **Modality dependence**: Further analysis showed that errors are more likely when entities lack image data, highlighting the importance of the visual modality despite its lower prevalence in the dataset.

2.19 Discussion and Future Work

Our comprehensive analysis of the dmg777k dataset and extensive experimentation with various multimodal GNN approaches has yielded several important insights:

- **Multimodal integration is key**: The most successful models effectively integrate information across modalities, confirming the value of multimodal approaches for knowledge graphs.
- **Pre-trained models provide strong foundations**: HuggingFace features consistently outperform simple features, demonstrating the value of leveraging pre-trained language and vision models.
- **Structure matters**: GraphSAGE's inductive bias is particularly well-suited for heterogeneous, multimodal knowledge graphs.
- **Adaptive sampling enables efficiency**: Our novel sampling approach successfully balances computational efficiency with model performance.
- **Fine-tuning improves domain adaptation**: Joint fine-tuning enhances performance by adapting pre-trained knowledge to domain-specific data.

3 Conclusion

In this project, we explored the challenging task of multimodal graph learning using the dmg777k dataset. We implemented a comprehensive pipeline that addresses multiple aspects of this problem:

- **Dataset exploration**: We conducted detailed exploratory data analysis to understand the structure and characteristics of the dmg777k knowledge graph.
- **Feature extraction**: We implemented multiple feature extraction approaches, from simple methods to advanced HuggingFace models.
- **Model development**: We created and evaluated several GNN architectures, including a specially designed MultiModalGNN with cross-modal attention.
- **Adaptive sampling**: We developed an innovative sampling strategy that dynamically adjusts based on training time and modality characteristics.
- **Joint fine-tuning**: We implemented and evaluated a CLIP-GNN model that jointly fine-tunes pre-trained vision and language models.

Our best model achieves 80.3% accuracy and an F1 score of 0.775 on the node classification task, demonstrating the effectiveness of our approach. The results confirm that effectively integrating multiple modalities in graph learning can significantly enhance performance on complex knowledge graph tasks.

This project contributes not only a high-performing model but also valuable insights into the challenges and opportunities of multimodal graph learning. The techniques and findings presented here can inform future research in this rapidly evolving field.

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