ALTeGraD 2023 Data Challenge

Molecule Retrieval with Natural Language Queries

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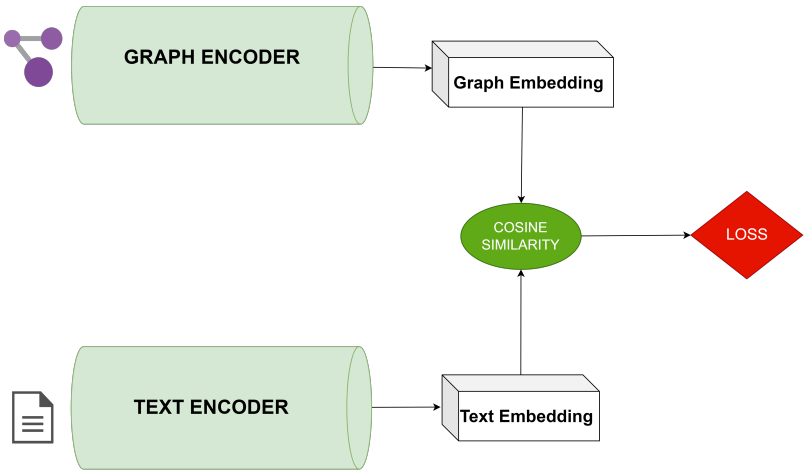
- Objective : Retrieve molecules from text queries.
- Challenge : Texts and molecules have different representations.
- Solution : Co-training framework.
  - Simultaneous training of text and molecule encoders.
  - Uses contrastive learning.
- Goal : Map similar text-molecule pairs closely, push dissimilar pairs apart.
- Outcome : Enhanced molecule retrieval from text queries.



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DistilBERT

- A distilled version of BERT, designed to be smaller and faster.
- Retains 97% of BERT's language understanding capabilities with 40% fewer parameters.
- Optimized for speed and efficiency, making it suitable for resource-constrained environments.

SciBERT [SciBERT : Pretrained Language Model for Scientific Text (Iz Beltagy et al., EMNLP 2019)]

- A variant of BERT trained on a large corpus of scientific text.
- Tailored for natural language processing tasks in the scientific domain.
- Improves performance on scientific datasets by better capturing domain-specific jargon and concepts.

- **Key Difference :** DistilBERT is a general-purpose, lightweight model, while SciBERT specializes in understanding scientific text.

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Text tokenizer :

- DistilBERT, SciBERT and SBERT were tested as text tokenizers
- In practice, SciBERT worked better in out experiments

Final text embdedding :

- The text tokenizer gives 768-dimensional embeddings
- Additional linear layer to reduce dimension to 350 (improve efficiency, and high enough to keep sufficient information)
- Normalization layer, so that embeddings obtained are more likely to match the one obtained by the graph encoder

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Different layers

1. **GCN (Graph Convolutional Networks)** : Integrates features from a node's neighbors, simulating convolutional operations on graphs.
2. **GAT (Graph Attention Networks)** : Applies attention over neighbors, prioritizing information flow from more relevant nodes.
3. **GIN (Graph Isomorphism Networks)** : Enhances sensitivity to graph's structural nuances, aiming at distinguishing non-isomorphic graphs.

Use of multiple layers :

1. 3 GCN layers (baseline model)
2. 3 GAT layers (best performance), 5 GAT layers (leads to overfitting)
3. Use of GCN, GAT and GIN independently and combine results (using mean)

We add a normalisation layer at the end.

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Contrastive loss (used in baseline model)

With logits $= v_1 \times v_2^T$, n the number of rows of logits,

labels $= \text{diag}(\text{range}(0, \text{logits.shape}[0])) = \begin{bmatrix} 0 & & \\ & \ddots & \\ & & n-1 \end{bmatrix}$ and CE the cross-entropy loss, we define the contrastive loss as follows :

$$\text{CL}(v_1, v_2) = \text{CE}(\text{logits}, \text{labels}) + \text{CE}(\text{logits}^T, \text{labels})$$

We also define the contrastive loss with temperature parameter :

$$\text{CL}_\tau(v_1, v_2) = \text{CE}\left(\frac{\text{logits}}{\tau}, \text{labels}\right) + \text{CE}\left(\frac{\text{logits}^T}{\tau}, \text{labels}\right)$$

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Negative contrastive loss [Text2Mol : Cross-Modal Molecule Retrieval with Natural Language Queries (Edwards et al., EMNLP 2021)]

With logits $= v_1 \times v_2^T$, eye $=$ diag_embed(labels) and BCEL the the Binary Cross-Entropy with Logits Loss, we define the negative sampling contrastive loss as follows :

$$\text{NegativeSamplingCL}(v_1, v_2, \text{labels}) = \text{BCEL}\left(\text{logits}, \text{eye}\right) + \text{BCEL}\left(\text{logits}^T, \text{eye}\right)$$

We also define the negative sampling contrastive with a temperature scaling parameter :

$$\text{NegativeSamplingCL}_\tau(v_1, v_2, \text{labels}) = \text{BCEL}(\frac{\text{logits}}{\tau}, \text{eye}) + \text{BCEL}(\frac{\text{logits}^T}{\tau}, \text{eye})$$

- We modified the dataloader to give triplets (text, graph, label) where $label = 1$ if the text and the graph are related to the same molecule, and $label = 0$ otherwise. In our training, we chose to have the same proportion (50%) of triplets with $label = 1$ and $label = 0$.
- With this loss, the model learns to differentiate matching pairs and non-matching pairs.
- Encourages the model to consider information from both text and graph.
- We used a trainable temperature scaling parameter.

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Cosine Embedding Loss

The Cosine Embedding Loss is defined as follows :

$$\text{CEL}(v_1, v_2, \text{label}, \text{margin}) = \begin{cases} 1 - \cos(v_1, v_2) & \text{if } \textit{label} = 1 \\ \max(0, \cos(v_1, v_2) - \text{margin}) & \text{if } \textit{label} = -1 \end{cases}$$

- We used the same dataloader as before

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Triplet Loss

The triplet loss is defined as follows :

$$\text{TripletL}(v, v_p, v_n, \text{margin}) = max(d(v, v_p) - d(v, v_n) + \text{margin}, 0)$$

In this loss we consider three embeddings :

- Embedding v associated to the graph of a certain molecule.
- Embedding v_p (called positive) linked to a text describing the previous molecule.
- Embedding v_n (called negative) linked to a text describing another molecule.

A custom Dataloader was created for this loss.

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Few words on computational resources :

- We were working with Google Colab and Kaggle.
- We used a batch size of 32 (couldn't increase it due to GPU limitations).
- Training time was between 6 and 30 hours (depending on architecture and number of epochs).

Training methods :

- Better results when we don't freeze any layers in training (we tried to freeze layers of the pre-trained text encoder).
- Best models obtained were trained on approximately 100 epochs.
- Learning rate was set to $2 \cdot 10^{-5}$ for the first epochs and gradually reduced to $1 \cdot 10^{-7}$.

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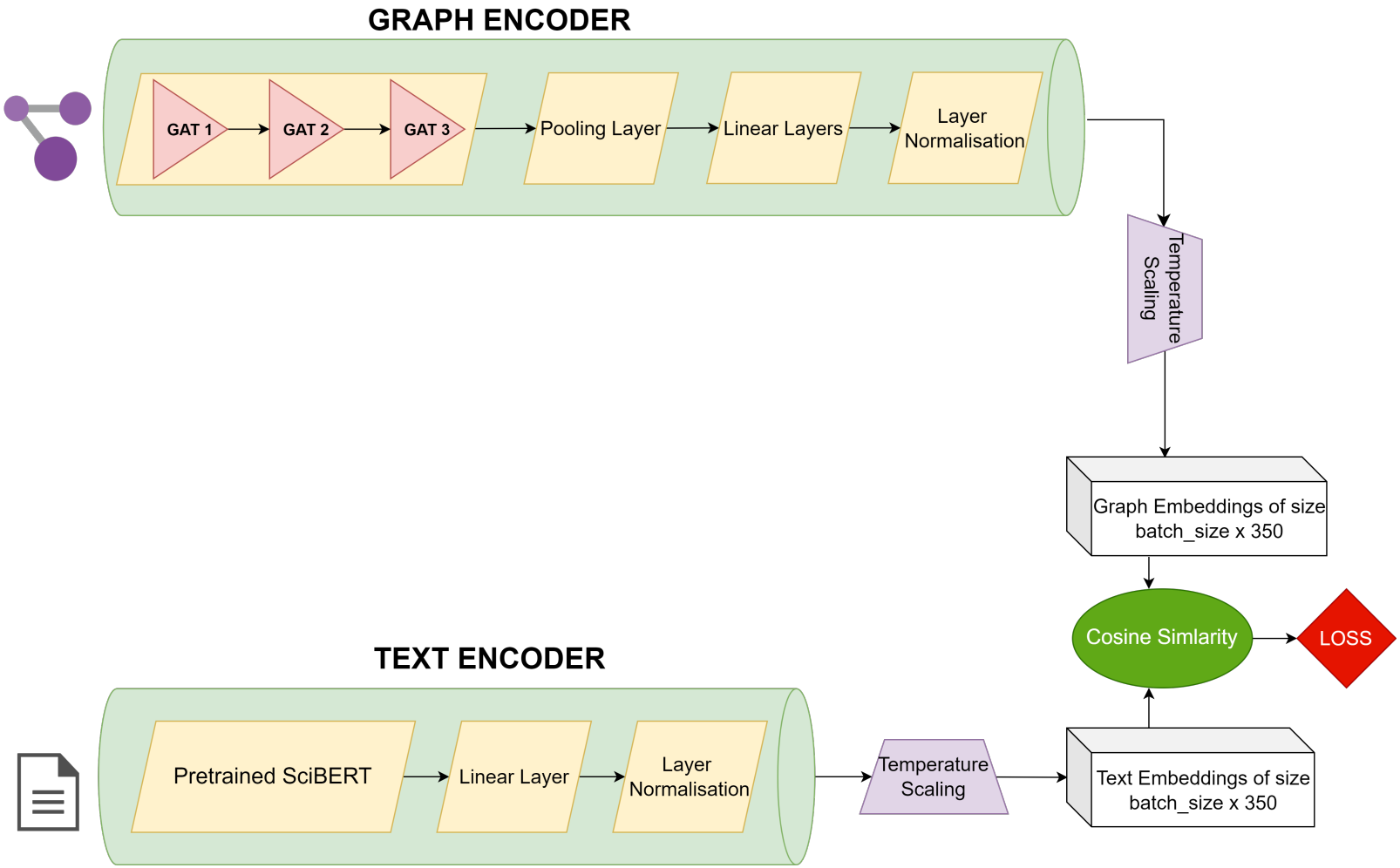

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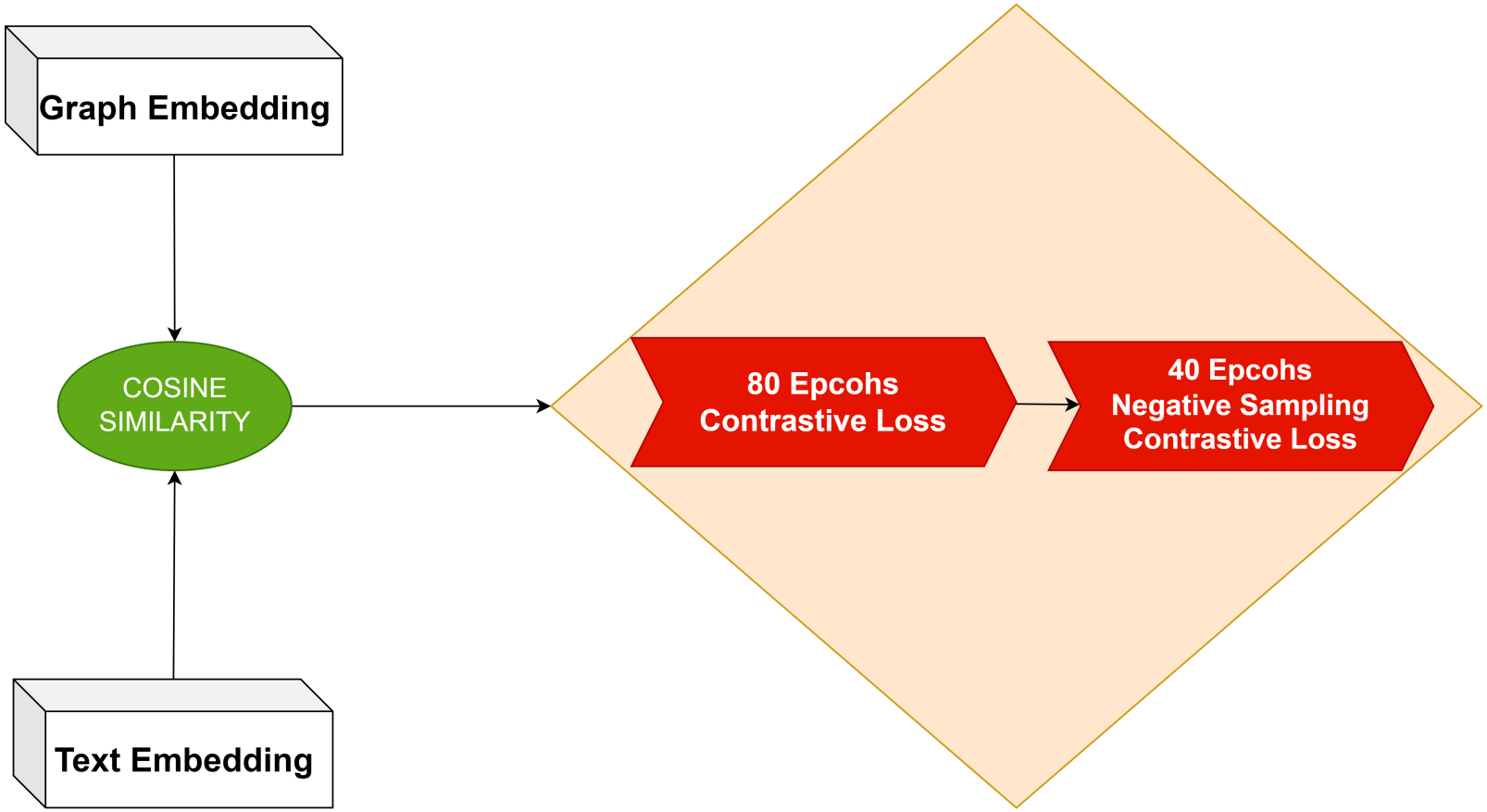

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Model Architecture				Loss				Train Setting		Result
Graph Enc.	Text Enc.	Out. Dim.	Temp. Scaling	Ctr. Loss	Neg. Sam.	Triplet Loss	Cos. Emb.	Epochs	Freeze Layers	Score
3 GAT	SciBERT	350	✓	✓	✓	X	X	120	X	0.87
3 GCN	SciBERT	350	✓	✓	✓	X	X	120	X	0.82
3 GAT	SciBERT	768	✓	X	✓	X	X	100	X	0.81
3 GAT	SciBERT	768	X	X	✓	X	X	60	X	0.79
5 GAT	SciBERT	768	X	X	✓	X	X	60	X	0.76
GCN+GAT+GIN	SciBERT	768	X	X	✓	X	X	60	X	0.74
3 GAT + 2 GCN	SciBERT	768	X	X	✓	X	X	50	X	0.71
3 GCN	SciBERT	768	X	✓	X	X	X	10	X	0.52
3 GAT	SciBERT	768	X	X	X	✓	X	50	X	0.46
3 GAT	SciBERT	768	X	X	X	X	✓	60	X	0.45
3 GCN	DistilBERT	768	X	✓	X	X	X	10	X	0.43
3 GCN	DistilBERT	768	X	✓	X	X	X	10	✓	0.4
3 GCN	SBERT	768	X	✓	X	X	X	20	X	0.38
3 GCN	SBERT	768	X	✓	X	X	X	20	✓	0.35

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What worked ?

1. Reducing the output dimension
2. Using contrastive loss then negative contrastive sampling loss
3. Use a temperature scaling parameter in the loss
4. Training on a large number of epochs
5. Using SciBERT as a text encoder
6. Using three GAT layers as a graph encoder
7. Changing the dataloader (generate in the same proportion positive and negative pairs)

What did not work ?

1. Using Triplet Loss (may require fine-tuning or selecting pairs)
2. Using too much (> 3) layers for graph encoder (didn't enhance performance and increase training time)
3. Using other graph encoders (GCN and GIN)

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- Co-training framework : Integrating SciBERT with a graph attention network for molecule retrieval from textual queries.
- Key observation : Choice of loss function crucial for results (Achieved 0.878 score).

Future avenues :

- Ensemble methods for model predictions.
- Experimentation with various loss functions.
- Parameter finetuning (e.g., scheduler, Triplet Loss margin).
- Initial use of Negative Sampling Contrastive Loss followed by Triplet Loss, or other combinaison of losses.