AI BIO INNOVATE CHALLENGE

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Problem Statement

PROBLEM STATEMENT

- Our project focuses on improving the field of organic chemistry by addressing a crucial aspect often overlooked—predicting the conditions necessary for chemical reactions during retrosynthetic analysis.
- Traditional methods rely on manual selection by experts, but we aim to automate this process using machine learning.
- Our approach involves building a seq2seq-based model using multitask learning that learns the relationship between reaction components and conditions.
- This innovation aims to accelerate synthesis planning, offering chemists a predictive tool to enhance efficiency and speed up chemical discovery.

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Data Processing

DATA PROCESSING

- Converting **SMILES** into molecular graphs for Graph Neural Networks involves using RDKit for featurization, converting SMILES to molecular objects, adding hydrogen atoms, and creating a graph with atom features and connectivity information.
- The conversion of **SMILES** to graph extends this by embedding the structure in 3D space, extracting features, and constructing an adjacency matrix.
- A mapping is generated to efficiently represent categorical data, assigning unique tokens random integers on first encounter and converted them into PyTorch tensor for compatibility with models.
- The PyTorch "Dataloader" class manages chemical reaction data using a DataFrame and a set sequence length.

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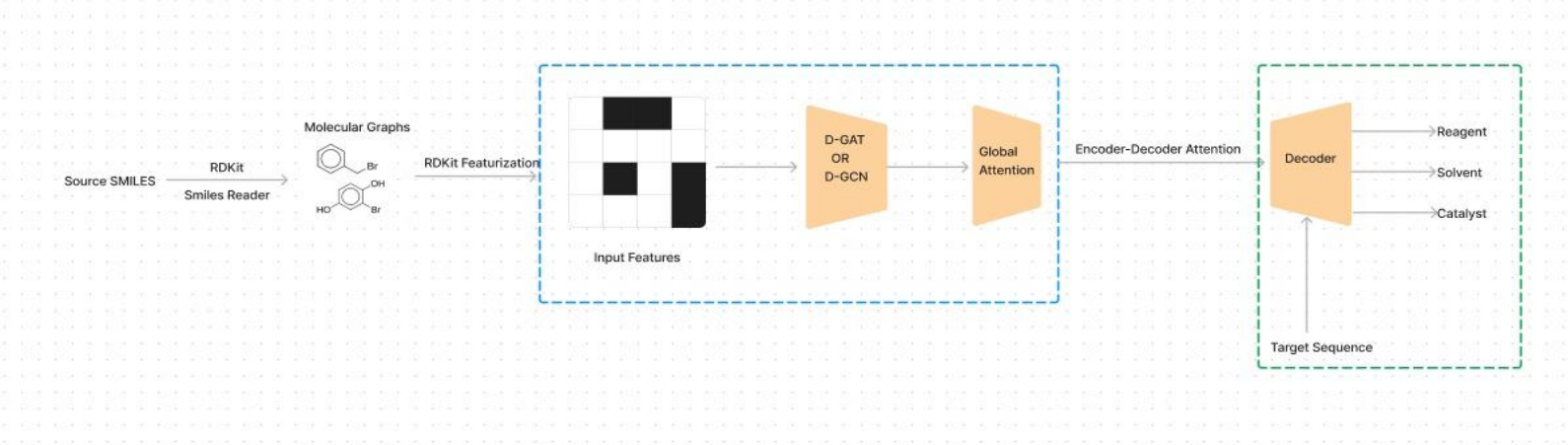
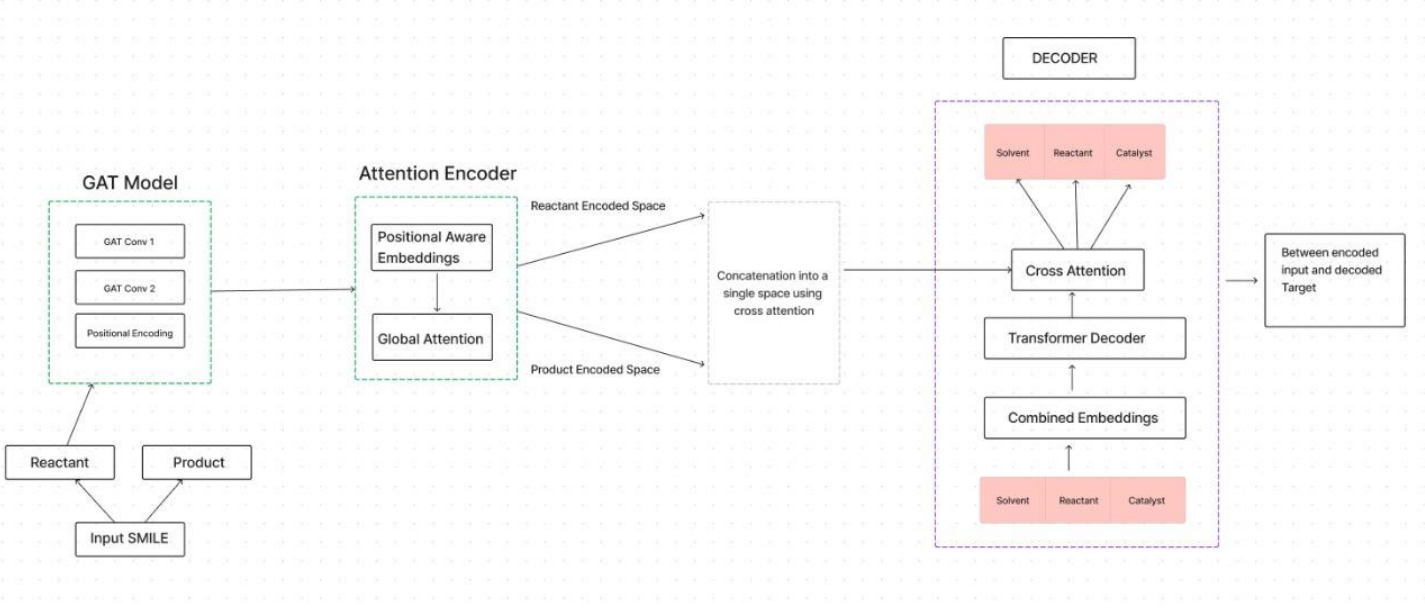
Methodology

Flow Of The Variables



- The source smiles are made into molecular graphs using RDKit after that we convert them to graph features which are parsed into our Graph Network followed by the Attention Encoder.
- The Decoder takes input of target sequence and concatenated with the encoder output by cross attention gives the probability output for each task.

Model Architecture



- The input SMILES are split into reactant and product, each fed separately into a GAT model with two layers. The model output is processed through an attention encoder, generating position-aware embeddings and applying global attention.
- In the decoder, the tasks are processed through a transformer decoder, cross-concatenated with the input sequence, and outputs are generated for three tasks using separate heads.

Inference

```
[32] o1,o2,o3=inference(model,'CC(C)(C)OC(=O)N1CC2CC(CN(Cc3ccccc3)C2)C1>>CC(C)(C)OC(=O)N1CC2CNCC(C2)C1')

     This is the original Reaction CC(C)(C)OC(=O)N1CC2CC(CN(Cc3ccccc3)C2)C1>>CC(C)(C)OC(=O)N1CC2CNCC(C2)C1 The reactant is  CC(C)(C)OC(=O)N1CC2CC(CN(C
     The Reagant of the original Reaction is phosphorus iodide ; 0 methanol|water water|platinum palladium iv water|platinum ammonium ethanol|nickel p
     The Solvent of the original Reaction is azide|cerium iodide|diisopropylamine
     The Catalyst of the original Reaction is iodide|diisopropylamine sodium peroxide|trifluoroacetic
```

- Here is the inference result, the input is a reaction in form of SMILES and below are the predicted reagent, solvent and catalyst. The output from the model is decoded to string using our mapping dictionary that we created

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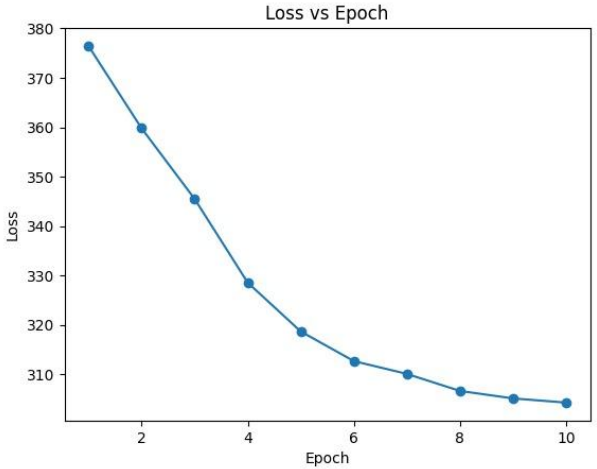
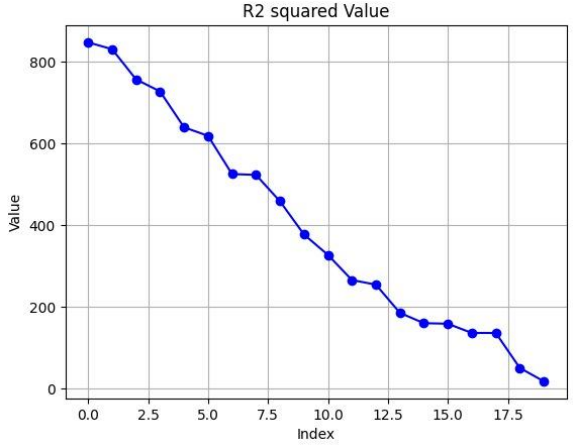
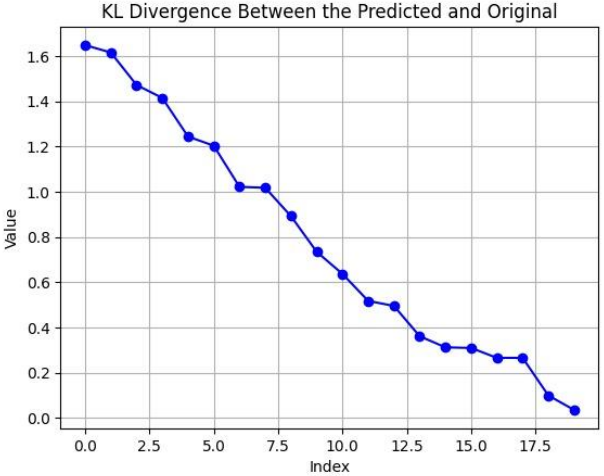
Evaluation Metrics



MSE LOSS



R2 Square



KL Divergence

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Future Scope

Future Scope

- A User Friendly Interface
- More Advanced mechanism for attentions
- Making a more Deeper Network
- Improving the Model Performance

Thank You