Progess of the Project

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Outline

- **GNN**
  - **Over-Sampling**
    - **Some Observation – Dimension, Embedding, Model**
    - **GraphSMOTE**
- **Future Work**

GNN - Oversampling

Oversampling

- Current Problem:
  - Can’t predict the edge in the small graphs consist of single triplet

	precision	recall	f1-score	support
T1003.003_9f73269695e54311dd61dc68940fb3e1	0.0	0.0	0.0	100.0
T1003.003_f049b89533298c2d6cd37a940248b219	0.0	0.0	0.0	100.0
T1007_c6607391-d02c-44b5-9b13-d3492ca58599	0.0	0.0	0.0	100.0
T1016_14a21534-350f-4d83-9dd7-3c56b93a0c17	0.0	0.0	0.0	100.0
T1016_71b3d2945679566b9d94d8cb11df4b70	0.0	0.0	0.0	100.0
T1016_921055f4-5970-4707-909e-62f594234d91	0.0	0.0	0.0	100.0
T1016_a0676fe1-cd52-482e-8dde-349b73f9aa69	0.0	0.0	0.0	100.0

```
Number of support=100: 54
Number of support=100 and f1-score<=0.2: 53
Number of support=100 and f1-score=0: 48
Number of support=200 and f1-score=0: 6
Number of support>200 and f1-score=0: 0
```

Oversampling

- Current Trial: hope to see the result on **training** dataset
  - At least let the model **overfit** first(remember the data with single triplet)
  - Use data with **320** times single triplet → # of training data = 13657600
  - Larger hidden **dimension** → more neurons to remember the data

- Hidden_dim = 256

```
Number of single triplet: 53
Number of single triplet and f1-score<=0.2: 0
Number of single triplet and f1-score<=0.5: 1
Number of single triplet and f1-score>0.5: 52

              precision    recall  f1-score   support

    accuracy                         0.70  16008233
   macro avg       0.80      0.79      0.79  16008233
weighted avg       0.71      0.70      0.70  16008233
```

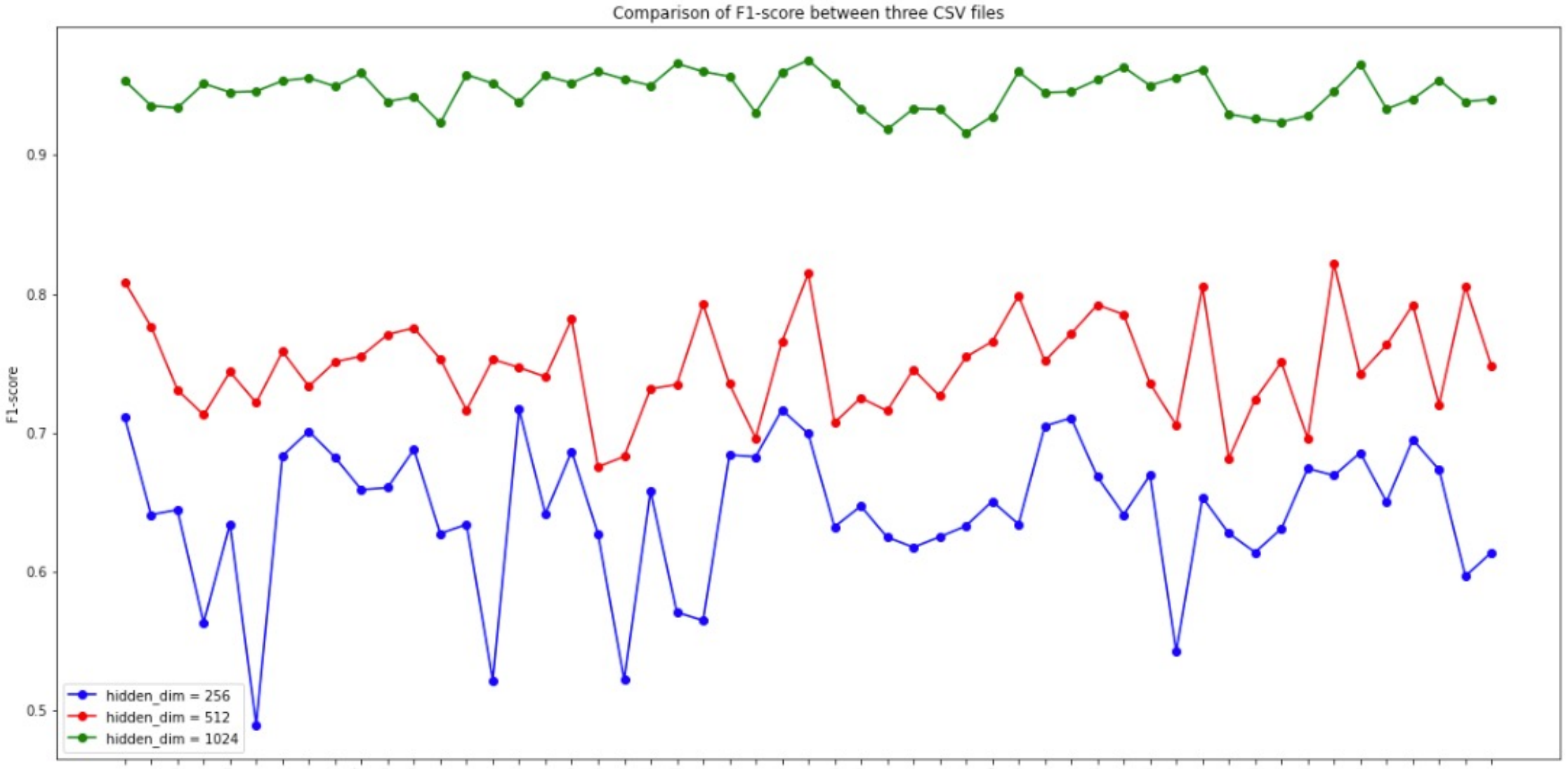
- Hidden_dim = 512

```
Number of single triplet: 53
Number of single triplet and f1-score<=0.2: 0
Number of single triplet and f1-score<=0.5: 0
Number of single triplet and f1-score>0.5: 53

              precision    recall  f1-score   support

    accuracy                         0.79  16008233
   macro avg       0.84      0.82      0.82  16008233
weighted avg       0.80      0.79      0.79  16008233
```

Experiment 3 - Oversampling



K-Fold Cross Validation

- Cross-validation should always be done **before** over-sampling the data, just as how feature selection should be implemented.
- Only by **resampling** the data repeatedly, **randomness** can be introduced into the dataset to make sure that there won't be an **overfitting** problem.

Training:

accuracy			0.99	12805285
macro avg	0.91	0.90	0.90	12805285
weighted avg	0.98	0.99	0.99	12805285

Testing:

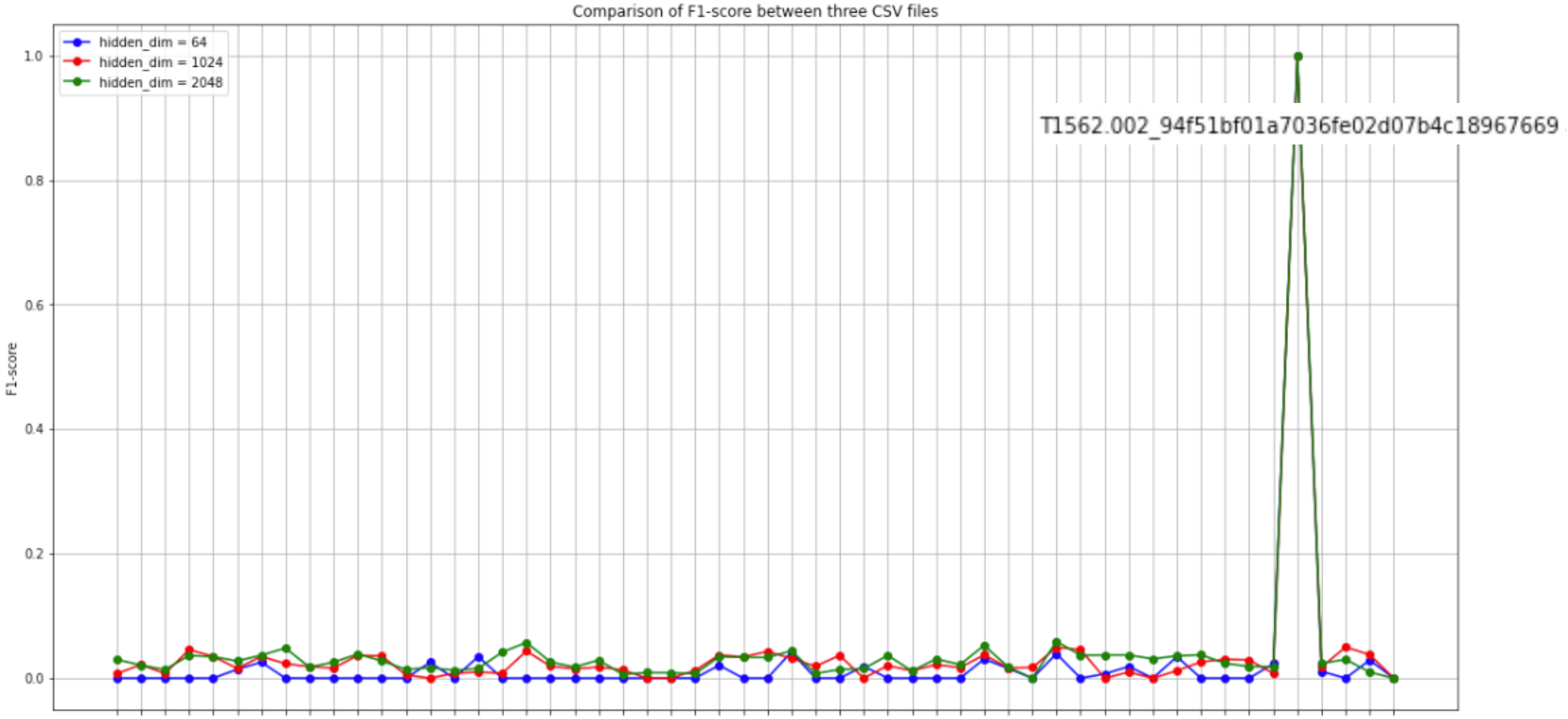
accuracy			0.97	310263
macro avg	0.60	0.59	0.59	310263
weighted avg	0.97	0.97	0.97	310263

Thoughts

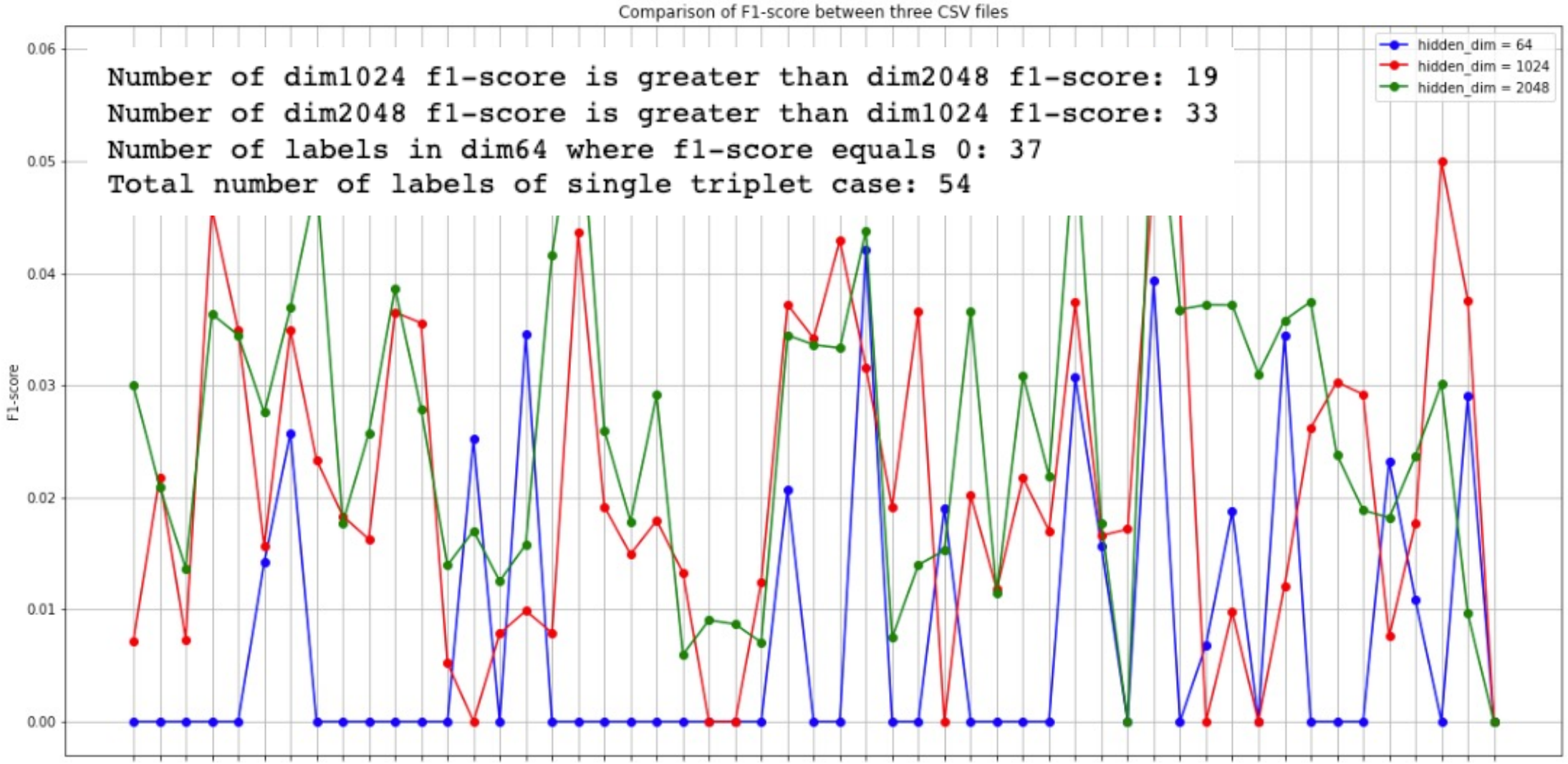
- Try the ensemble
  - Different GNN
    - Different **hidden dimension**
    - Different **embedding**
    - Different **model**

  - Different type of model → **MLP, RNN, GNN…**
    - Maybe the different can identify the different single triplet class

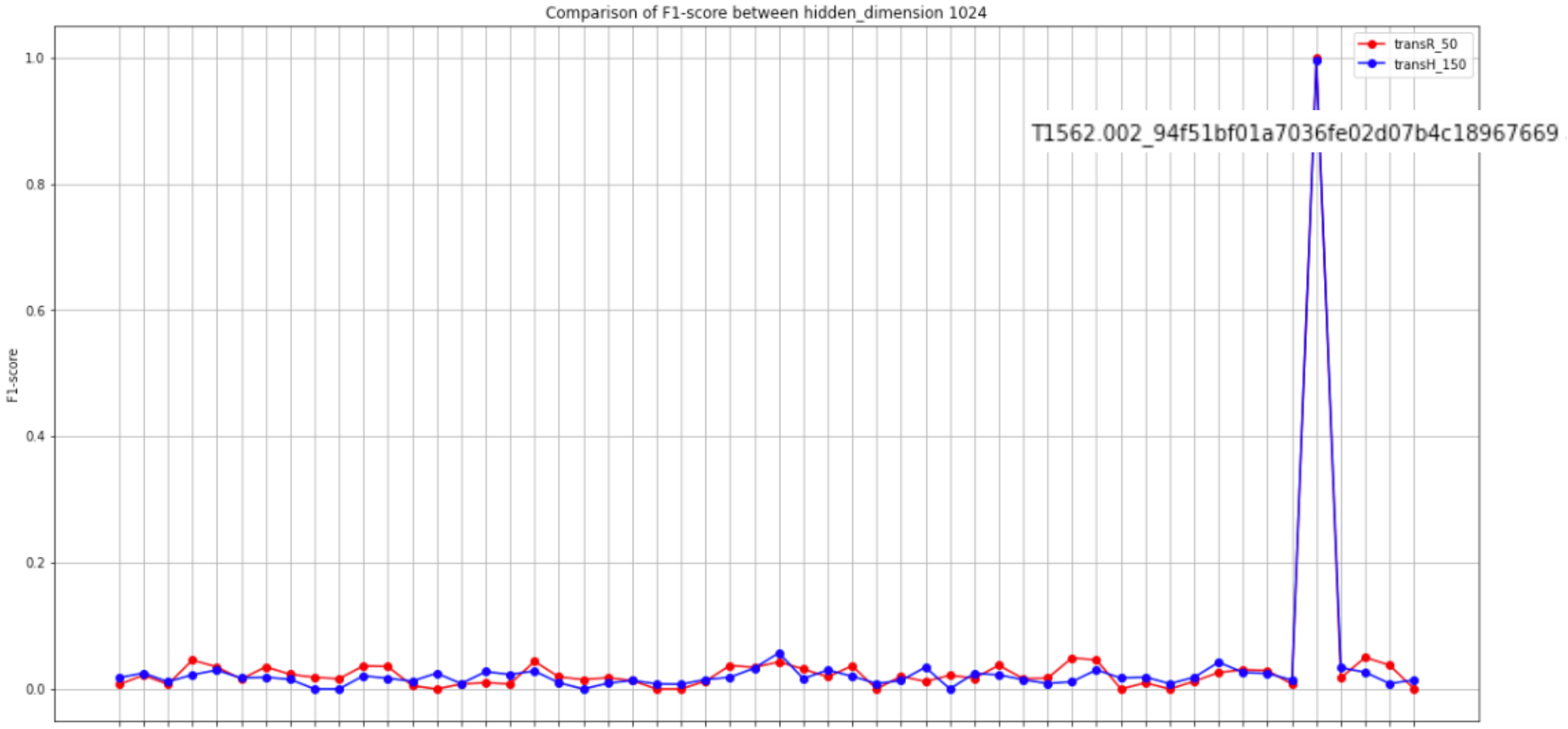
Observation on Different Dimension



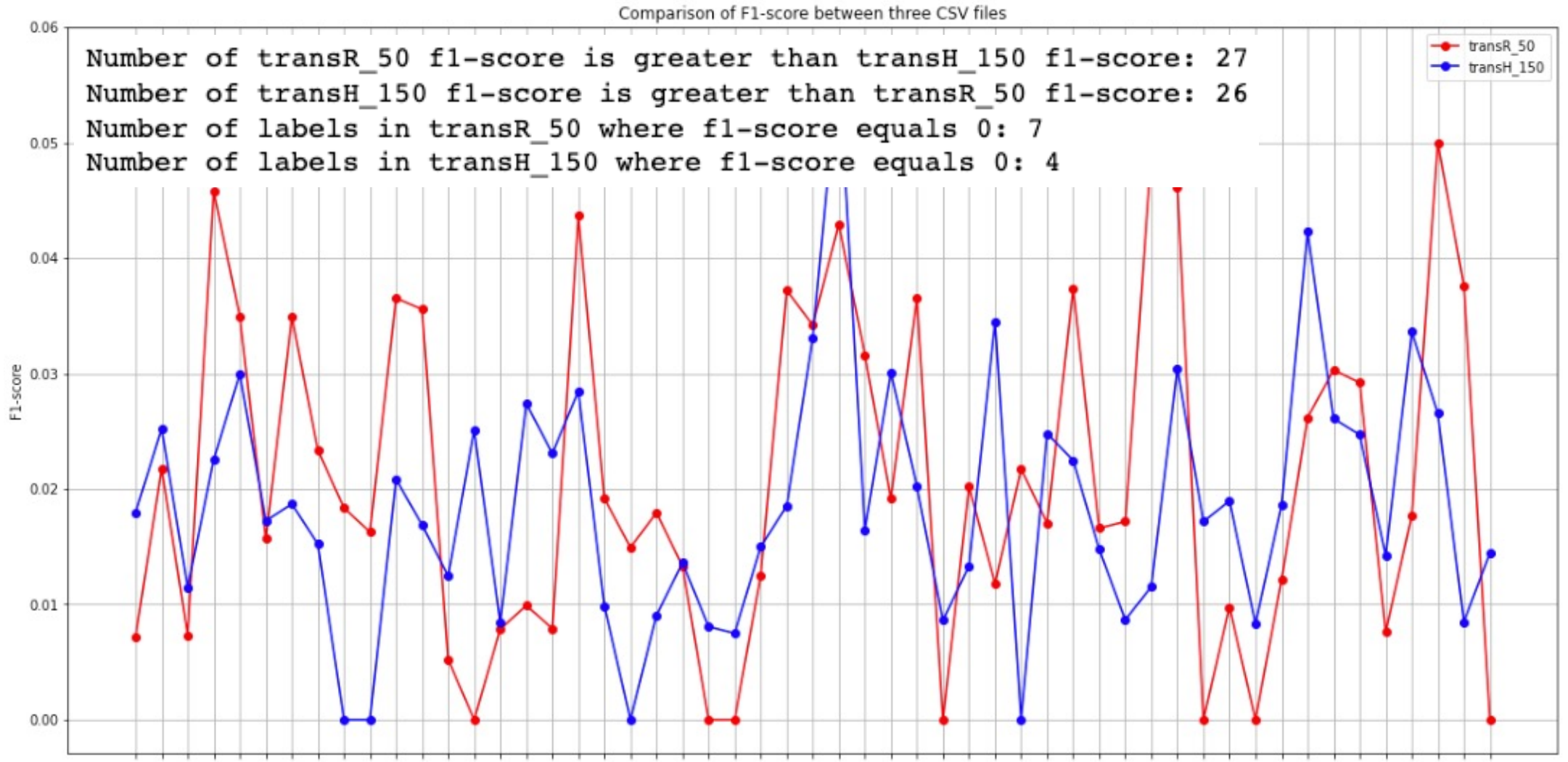
Observation on Different Dimension



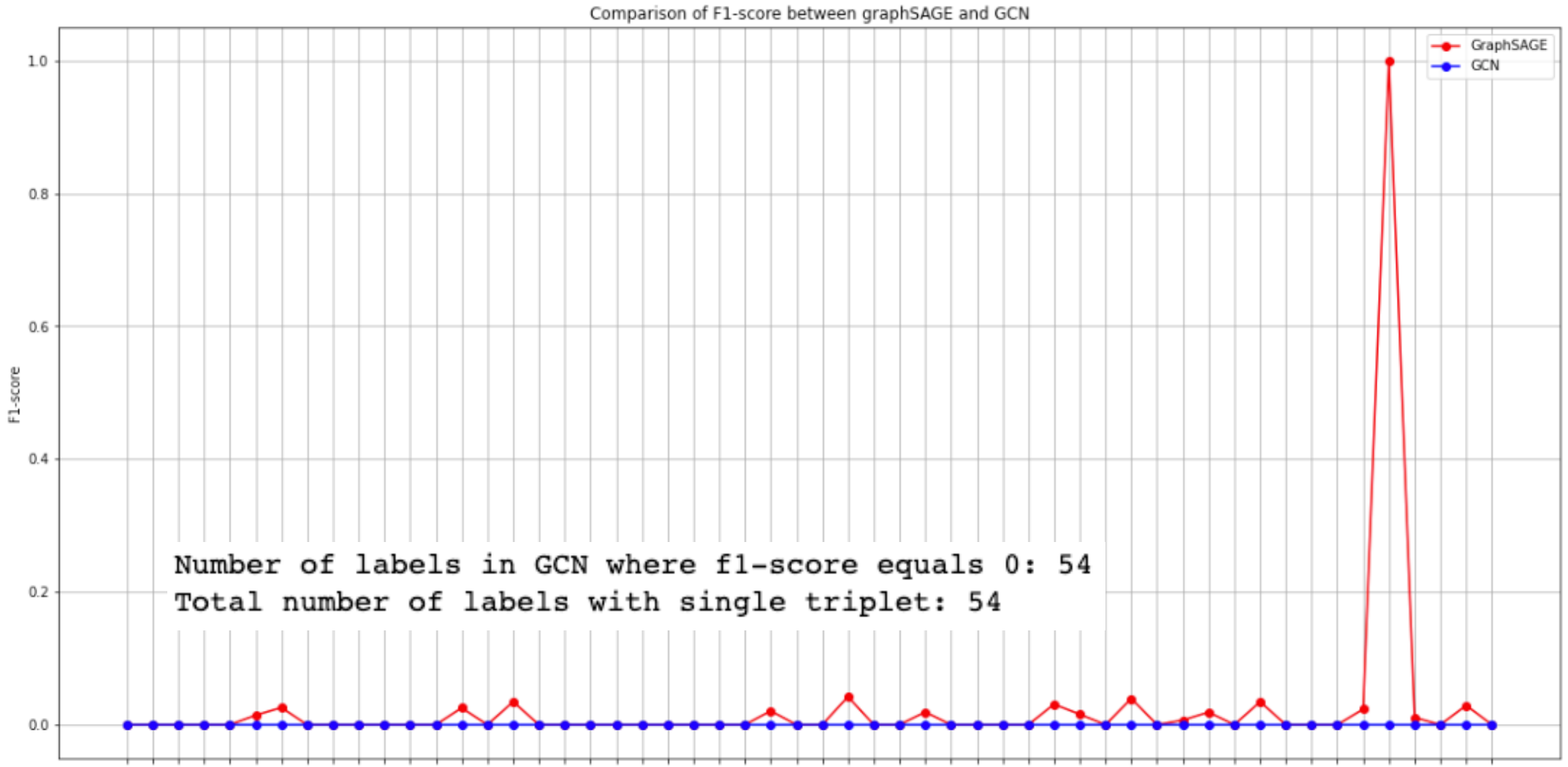
Observation on Different Embedding



Observation on Different Embedding



Observation on Different Model



Observation

- Noticed that **T1562.002_94f** always got predicted in all the experiments
  - What if MLP and RNN can detect different class?
  - After Euni give me the **MLP** and **RNN** model, I'll observe the results of them

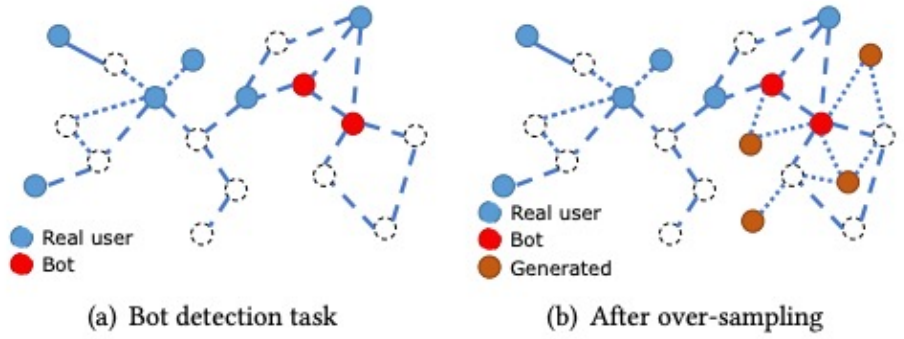
- **Hidden Dimension** do have an effect on the result → but it's all about from 0 to 0.05
- **Embedding** (transR_50 and tansH_150) seems to have the similar result → try more
- My GCN test sucks → try GAT or other GNN model

GraphSMOTE

GraphSMOTE: Imbalanced Node Classification on Graphs with Graph Neural Networks

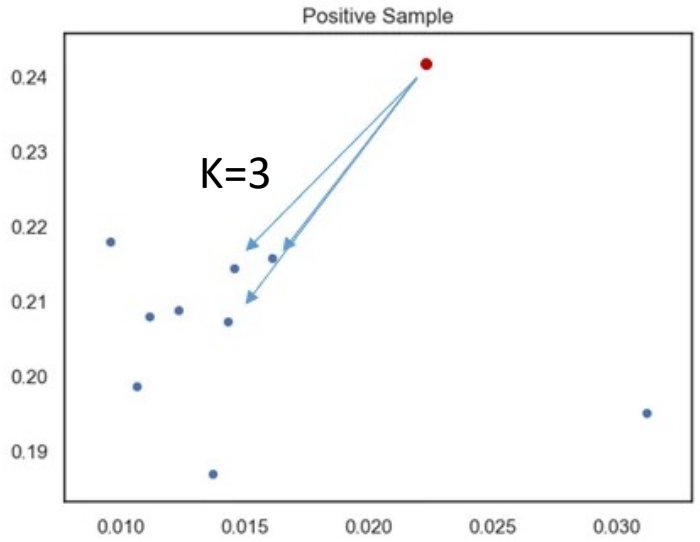
WSDM '21, March 8–12, 2021, Virtual Event, Israel

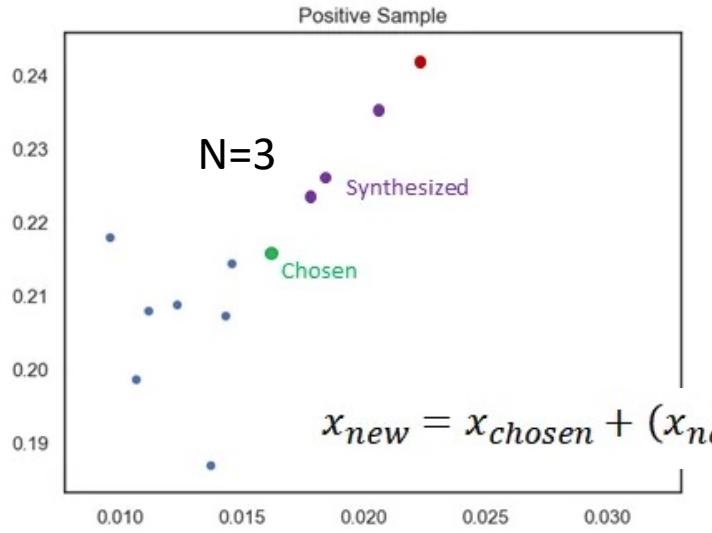
Tianxiang Zhao, Xiang Zhang, Suhang Wang



(a) Bot detection task (b) After over-sampling

- **Synthesized Minority Oversampling Technique (SMOTE)**





$$x_{new} = x_{chosen} + (x_{nearest} - x_{chosen}) * \delta\,;\ \delta \in [0,1]$$

Future Work

Future Work

- **GNN**
  - Try some other methods to improve the performance of single triplet issue
    - Figure out why the model can detect the **T1562.002_94f**
    - Try to ensemble if the **MLP** and **RNN** model's result are different
    - Read the **GraphSMOTE** paper
    - Try some other embeddings?
    - Try some other models?
    - Try some data augmentation methods?
    - …

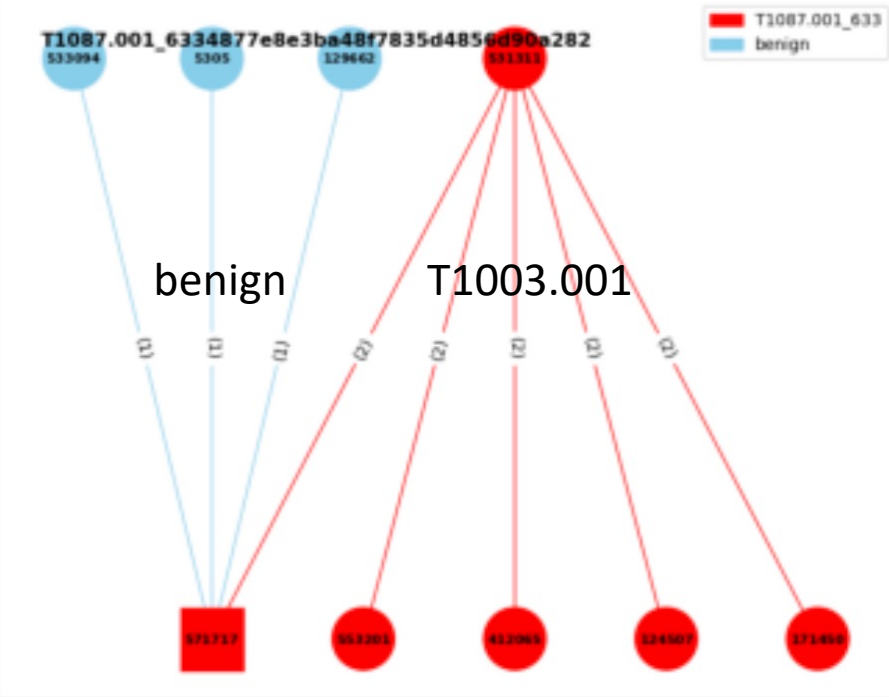
Thanks!!

Appendix

Experiment 3

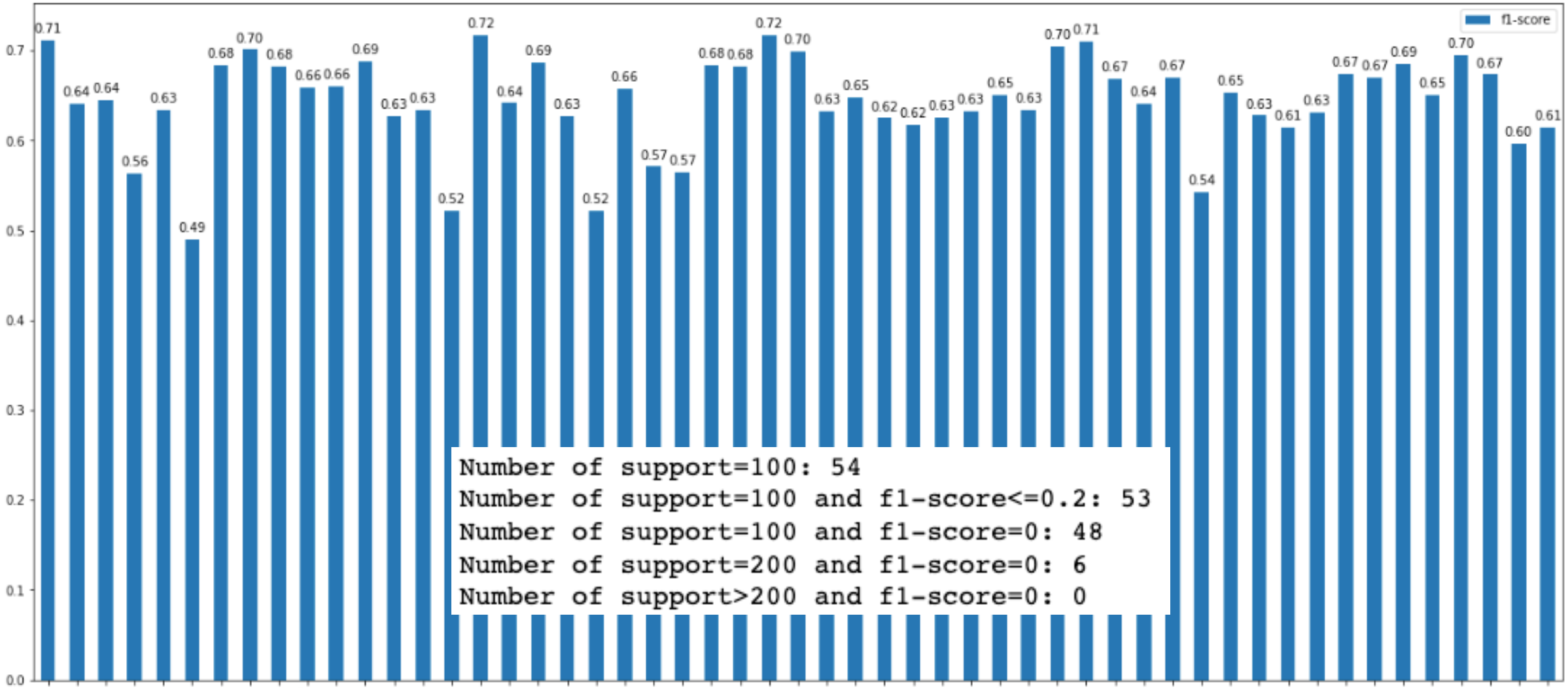
- **Experiment 3:**
  - Consider the **neighbor** benign nodes
  - Edge classification

  - Given a graph → label the triplets with the benign or the specific AP



Experiment 3 - Oversampling

Bar Chart of hidden dimension = 256:



Experiment 3 - Oversampling

- Current Trial: Duplicate the data with single triplets → 20, 40, 80, 320 times

20 times

```
Number of support=100: 54
Number of support=100 and f1-score<=0.2: 53
Number of support=100 and f1-score=0: 21
Number of support=200 and f1-score=0: 10
Number of support>200 and f1-score=0: 1
```

accuracy	0.971560	0.971560	0.971560	0.97156
macro avg	0.597445	0.600577	0.594684	310263.00000
weighted avg	0.970613	0.971560	0.970482	310263.00000

40 times

```
Number of support=100: 54
Number of support=100 and f1-score<=0.2: 53
Number of support=100 and f1-score=0: 14
Number of support=200 and f1-score=0: 10
Number of support>200 and f1-score=0: 2
```

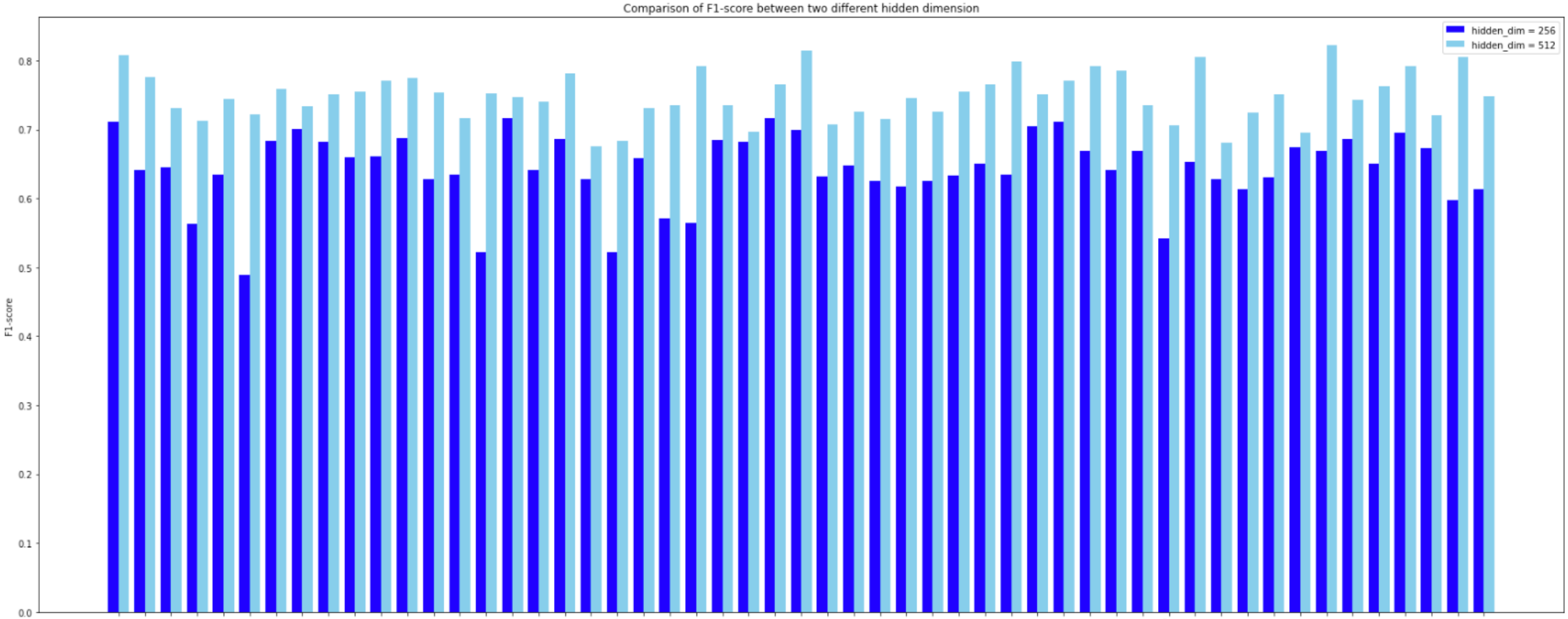
accuracy	0.971318	0.971318	0.971318	0.971318
macro avg	0.602542	0.597866	0.594387	310263.000000
weighted avg	0.971349	0.971318	0.970477	310263.000000

80 times

```
Number of support=100: 54
Number of support=100 and f1-score<=0.2: 53
Number of support=100 and f1-score=0: 18
Number of support=200 and f1-score=0: 10
Number of support>200 and f1-score=0: 3
```

accuracy	0.971463	0.971463	0.971463	0.971463
macro avg	0.596490	0.598077	0.594237	310263.000000
weighted avg	0.970626	0.971463	0.970567	310263.000000

Experiment 3 - Oversampling



Experiment 3 - Model

- Concept from the DGL official website:
  1. Let the dgl graph's edge data have the attribute: **edata["label"]**
  2. Use **GraphSAGE** model to get the new **node embedding**
  3. Use **MLP** model to get the **score** of the edge
  4. Concatenate these two models
  5. Train the final model

```
g.ndata['feat'] = th.tensor(data["node_feat"])
g.edata['feat'] = th.tensor(data["edge_attr"])
g.edata['label'] = th.tensor(data["labels"])
```

```
def model_fn(batched_g, model, criterion, device, count=1, which_type='train'):
    """Forward a batch through the model."""
    batched_g = batched_g.to(device)
    labels = batched_g.edata['label'].to(device)

    logits = model(batched_g, batched_g.ndata['feat'].float())
    loss = criterion(logits, labels)

    output = torch.softmax(logits, dim=1)
    preds = output.argmax(1)

    accuracy = torch.mean((preds == labels).float())
```

Experiment 3 - Model

```python
class GraphSAGE(nn.Module):
    def __init__(self, in_dim, hidden_dim, out_dim):
        super(GraphSAGE, self).__init__()
        self.layer1 = dglnn.SAGEConv(in_dim, hidden_dim, 'pool')
        self.layer2 = dglnn.SAGEConv(hidden_dim, out_dim, 'pool')

    def forward(self, g, inputs):
        h = self.layer1(g, inputs)
        h = torch.relu(h)
        h = self.layer2(g, h)
        return h
```

```python
class MLPPredictor(nn.Module):
    def __init__(self, out_feats, out_classes):
        super().__init__()
        self.W = nn.Linear(out_feats*2, out_classes)

    def apply_edges(self, edges):
        h_u = edges.src['h']
        h_v = edges.dst['h']
        score = self.W(torch.cat([h_u, h_v], 1))
        return {'score': score}

    def forward(self, graph, h):
        with graph.local_scope():
            graph.ndata['h'] = h
            graph.apply_edges(self.apply_edges)
            return graph.edata['score']
```

```python
class Model(nn.Module):
    def __init__(self, in_features, hidden_features, out_features, num_classes):
        super().__init__()
        self.sage = GraphSAGE(in_features, hidden_features, out_features)
        self.pred = MLPPredictor(out_features, num_classes)

    def forward(self, g, node_feat, return_logits=False):
        h = self.sage(g, node_feat)
        logits = self.pred(g, h)

        return logits
```

Experiment 3 - Result

- **Format of the edge labels:**
  - Label 65 is benign

```
labels of Test: tensor([155,  65, 155, 155, 155], device='cuda:0') torch.Size([5])
predicted of Test: tensor([155,  65, 155, 155, 155], device='cuda:0') torch.Size([5])
labels of Test: tensor([61, 61, 61], device='cuda:0') torch.Size([3])
predicted of Test: tensor([61, 61, 61], device='cuda:0') torch.Size([3])
```

- **Classification report**:
  - transR_50:

4a0dc2e1f5d1a	0.00	0.00	0.00	100
167175e8a019a	1.00	1.00	1.00	800
c3579e9e3737b	1.00	1.00	1.00	6200
43d838e0791ca	1.00	1.00	1.00	600
benign	1.00	1.00	1.00	134563
accuracy			0.97	310263
macro avg	0.60	0.61	0.60	310263
weighted avg	0.97	0.97	0.97	310263

  - secureBERT_50:

714a0dc2e1f5d1a	0.00	0.00	0.00	100
fb167175e8a019a	0.98	1.00	0.99	800
2ac3579e9e3737b	0.97	0.98	0.98	6200
0243d838e0791ca	0.91	0.83	0.87	600
benign	0.99	1.00	0.99	134563
accuracy			0.92	310263
macro avg	0.52	0.48	0.49	310263
weighted avg	0.90	0.92	0.91	310263

  - **Macro average** is similar to previous experiments → won't be affected by benign
  - **Weighted average** is very high since the # of the benign is high(unbalanced) and predictable
  - TransX family performs better than secureBERT

Experiment 3 – Noise

- Current Trial 1:
  - Add the **noise** to the node feature

```
def collate(samples):
    data_list = samples
    batched_graphs = []
    for data in data_list:
        g = dgl.graph((th.tensor(data["edge_index"][0]), th.tensor(data["edge_index"][1])), num_nodes=data["num_nodes"]

        node_feat = th.tensor(data["node_feat"])

        noise = th.normal(mean=0, std=0.01, size=node_feat.shape, device=node_feat.device)
        node_feat += noise

        g.ndata['feat'] = node_feat
        g.edata['feat'] = th.tensor(data["edge_attr"])
        g.edata['label'] = th.tensor(data["labels"])  # Add edge labels to graph

        batched_graphs.append(g)

    return dgl.batch(batched_graphs)
```

```
Number of support=100: 54
Number of support=100 and f1-score<=0.2: 53
Number of support=100 and f1-score=0: 46
Number of support=200 and f1-score=0: 4
Number of support>200 and f1-score=0: 0
```

Experiment 3 – K-fold validation

k-fold cross-validation（k 折交叉驗證）是一種在機器學習中常用的模型評估方法，尤其在有限的數據集上評估模型性能時非常有效。其主要優點包括：

1. **更可靠的性能估計**：通過將數據集分成 k 個子集，每次使用其中一個子集作為測試集，其餘 k-1 個子集作為訓練集，然後重複此過程 k 次，每次選擇不同的子集作為測試集，可以使得模型評估的結果更加穩定和可靠。
2. **充分利用數據**：每個數據點都被用作 k-1 次的訓練和 1 次的測試，這意味著每個數據點都被充分利用，這在數據量不大時尤其重要。
3. **減少偏差**：由於模型需要在 k 個不同的訓練集上訓練，然後在 k 個不同的測試集上測試，這有助於降低模型在特定數據集上的性能估計偏差。
4. **更好的泛化性能評估**：通過對不同的訓練集和測試集進行訓練和測試，可以幫助評估模型對未見數據的泛化能力。
5. **減少過擬合風險**：k-fold cross-validation 有助於識別模型是否對特定的訓練數據集過度擬合，因為它必須在多個不同的訓練集上表現良好。

然而，k-fold cross-validation 也有其局限性，例如計算成本較高（尤其是 k 較大和模型訓練時間較長時），並且結果可能依賴於 k 的選擇以及數據分割的方式。這些都是在使用此方法時需要考慮的因素。