

Successful Contrastive Pretraining of Set Transformer

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Computational Finance

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Introduction

- Transformer - To process long sequences of data in NLP.
- Vision Transformer - Processes images by creating patches and the corresponding vector.
- Set Transformer - A permutation invariant model to process unordered sets, which is independent of positional embeddings makes it permutation equivariant, in contrast to Transformer and Vit.
- Contrastive Learning with Set Transformer - a unique approach to enhance the Set Transformer performance, which has been successfully contributed in Transformer and Vision Transformer models.
- Generalization
 - Weak generalization
 - Strong generalization



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Data

- Point cloud 3D Body scan
- Collected by Dr. Frederick Steven Cottle
- KX-16 Body Scanner [1]
- Dataset includes 75 Participants' unlabeled (unavailable metadata) data files, with point cloud count ranging between 51000 to 63000.
- As a preliminary step, this unlabelled dataset is used for the classification, a self-identifying task.



Data

- Figure 1 shows the initial body scan, train to validation split of point clouds, and subsampling during each batch iteration.

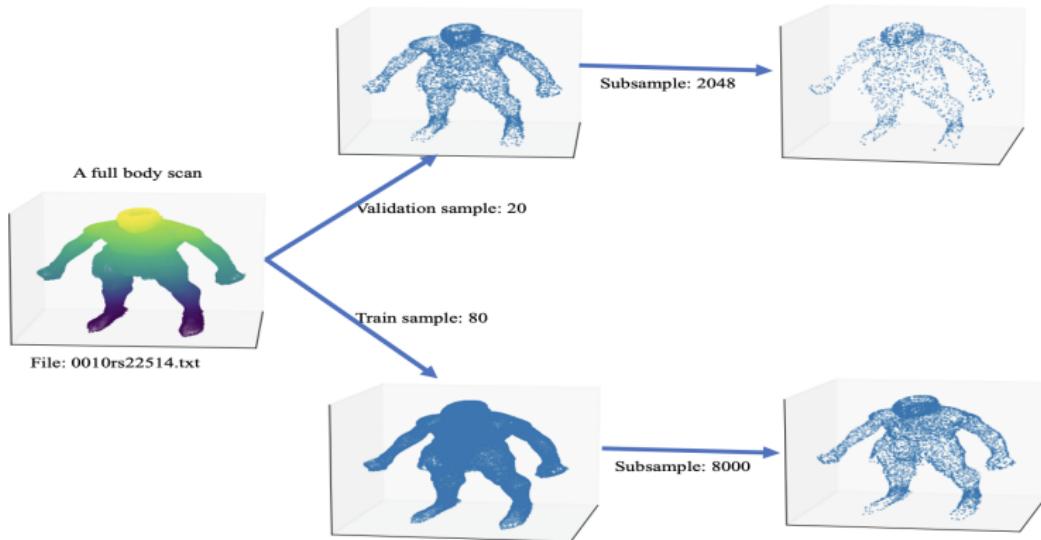


Figure 1: Point cloud 3D Body Scan flow to train and validate on subsample



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Background

- Set Transformer - Lee, J. et. al. (2018) [2]
 - Induced Set Attention Block(ISAB) - speeds up computation ($\mathcal{O}(nm)$) and extracts meaningful features.
 - Pooling layer - parameterized aggregation function, helps to capture the varying contribution of the instances, for better aggregation. Pooling by attention operation makes the model permutation invariant.

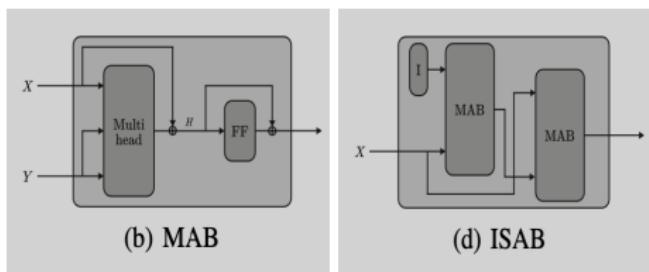


Figure 2: Multi Head Attention Block(MAB)[2]

Figure 3: Induced Set Attention Block(ISAB)[2]

Background

- Simple framework for Contrastive Learning [3] - Chen, T. et. al. (2020): ResNet-50 on ImageNet dataset, Positive pair/ Negative pair. Using SimCLR self-supervised method shows similar performance to Resnet-50 supervised learning.
- Generalization
 - Kullback-Leibler divergence(KL divergence) [4]

$$D_{KL}(P||Q) = \sum_{x \in X} P(x) \log \left(\frac{P(x)}{Q(x)} \right) \quad (1)$$



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Methods

General Experimental Setup

- Data Loader
- Batch size - train:4, validation:4
- Sub sample size - train:8000, validation:2048
- Train : Validation = 80:20
- Monte Carlo Simulation - 10
- Optimizer - Adam
- Loss - Sparse categorical cross entropy



Experimental Setup

Hyperparameters

Standard Set Transformer

Embedded dimensions - 64, 32
Number of heads - 32, 16
Induce points - 128, 64
stack - 3
Dropout - 0.05
Learning rate - 1e-03
Number of epochs - 250

Contrastive Pretraining

Experimented batch size - 32, 16
Point cloud - 1024, 2048
Temperature - 0.5
Number of epochs - 200

Fine Tuning

Linear layer - 128, 1024
Non-linear activation function - LeakyReLU
Dropout - 0.1
The rest of the hyperparameters are
maintained as same as Standard Set Transformer



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Standard Set Transformer Algorithm

Set Transformer architecture

```
1:  $y = \text{Linear}(3, \text{embed\_dim})$ 
2: for  $j = 1$  to  $\text{stack}$  do
3:    $y = \text{InducedSetAttentionBlock}(y)$ 
4: end for
5:  $y = \text{Dropout}(0.05)(y)$ 
6:  $y = \text{PoolingByMultiHeadAttention}(y)$ 
7:  $y_{\text{embedding}} = \text{Dropout}(0.05)(y)$ 
8:  $y = \text{FinalDense}(\text{numberofclasses})(y_{\text{embedding}})$ 
9: return  $y, y_{\text{embedding}}$ 
```



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Contrastive Learning using Set Transformer

Visual representation of contrastive learning

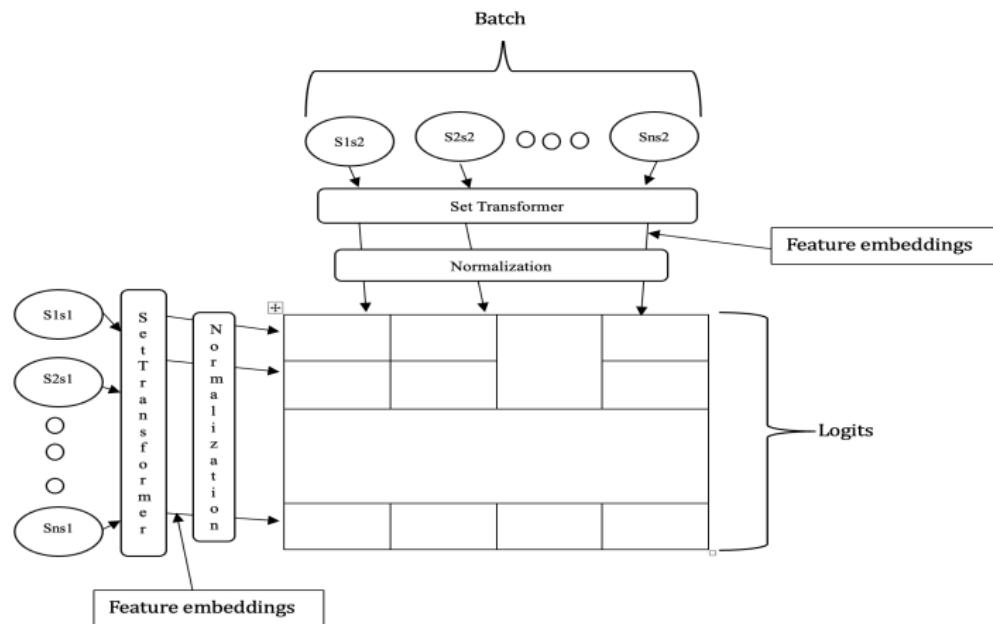


Figure 4: Contrastive Learning using Set Transformer architecture



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Contrastive Learning using Set Transformer

Algorithm

Contrastive Learning architecture

```
1:  $y_1, y\_embedding1 = \text{SetTransformer}(\text{batch1})$ 
2:  $y_2, y\_embedding2 = \text{SetTransformer}(\text{batch2})$ 
3:  $y\_embedding1 = \text{Linear}(\text{embed\_dim}, \text{projection\_dim})(y\_embedding1)$ 
4:  $y\_embedding2 = \text{Linear}(\text{embed\_dim}, \text{projection\_dim})(y\_embedding2)$ 
5:  $y\_embedding1 = \text{Norm}(y\_embedding1)$ 
6:  $y\_embedding2 = \text{Norm}(y\_embedding2)$ 
7:  $y = \text{Mul}(y\_embedding1, y\_embedding1.T) * \text{Temperature}$ 
```



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Generalization

- Weak Generalization - Has knowledge about all the category data at the time of training.
- Strong Generalization(leave one out) - Is not aware of a particular class data at a given training period.
- Probability matrix - 75×75
- Reassign all diagonal elements in weak generalization 0.
- Normalize both of the matrices
- Apply KL Divergence



Visualization

- Get feature embeddings for both standard Set transformer and Contrastive pre-trained model.
- 10 vectors for each sample.
- Applied PCA with 2 principal components to visualize in 2D.
- Applied t-SNE with a 2D component with the perplexity of 20.
- Evaluate along the 2D axis if, distribution is relatable to human distinguish.



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Results



Standard Set Transformer

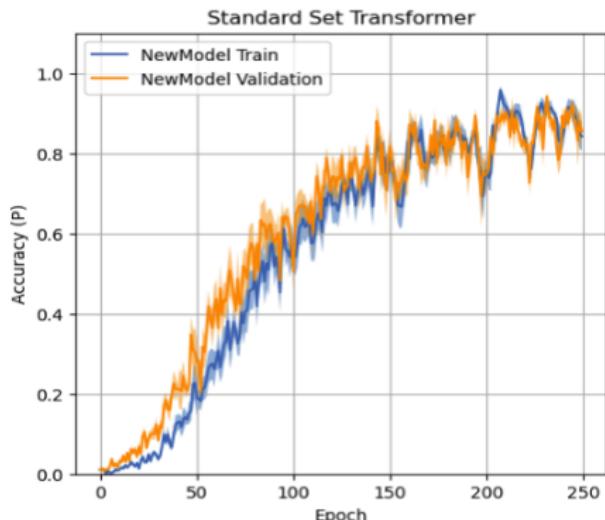
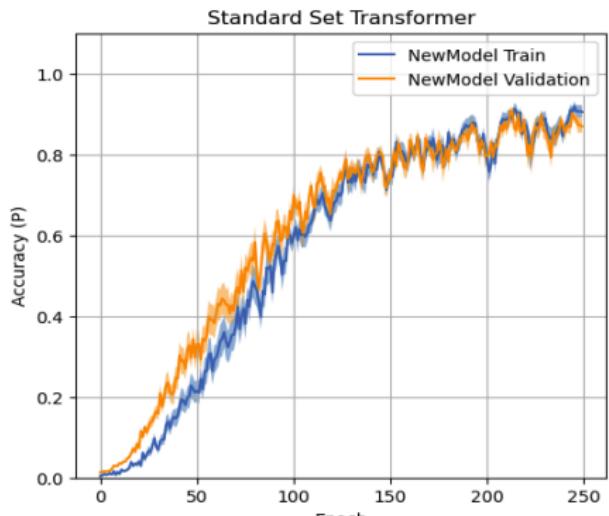


Figure 5: Monte Carlo simulated Standard Set Transformer Accuracy

Contrastive Learning using Set Transformer

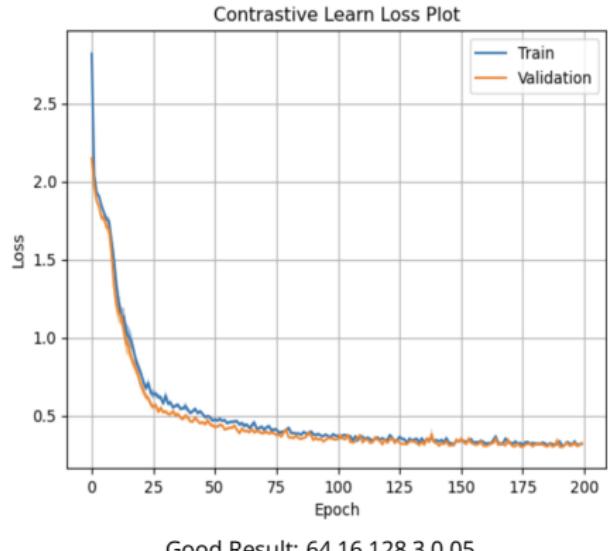
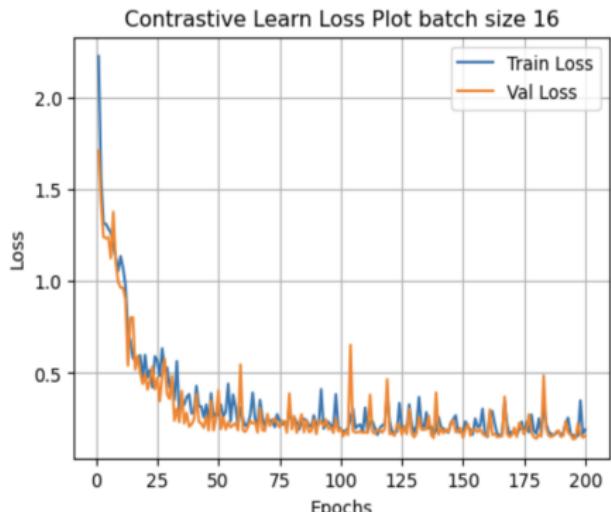


Figure 6: Monte Carlo simulated Contrastive Learning using Set Transformer Loss

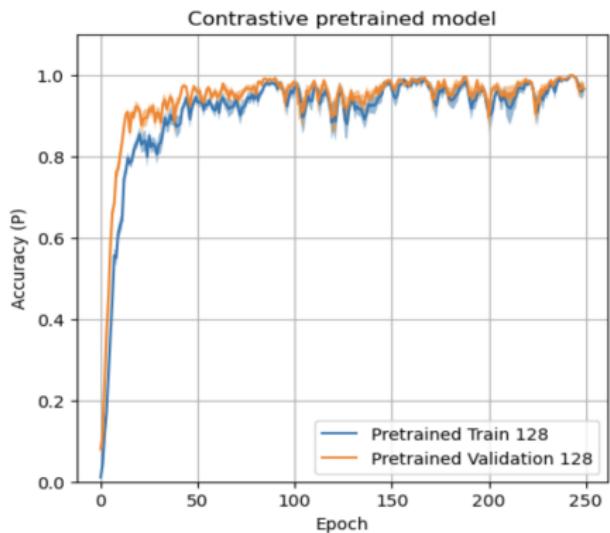


Bad Result: 64,16,128,3,0.05,batch size: 16

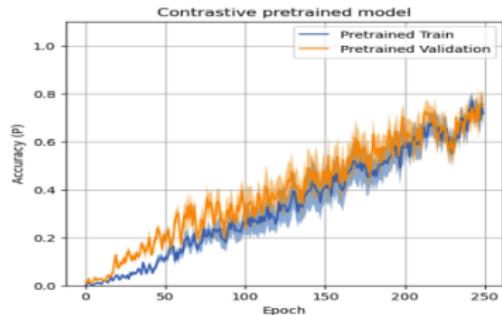


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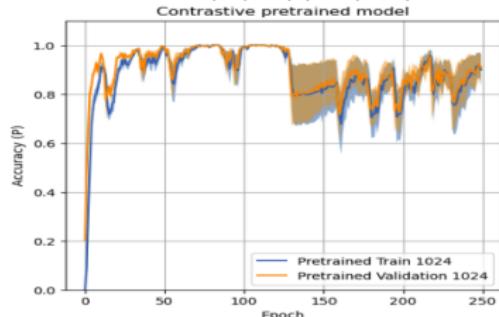
Fine Tuning



Good Result: 64,16,128,3,0.05, 128, 0.1



Bad Result: 64,32,128,3,0.05, 128, 0.1



Bad Result: 64,16,128,3,0.05, 1024, 0.1

Figure 7: Monte Carlo simulated Contrastive pre-trained model Accuracy



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Weak Generalization

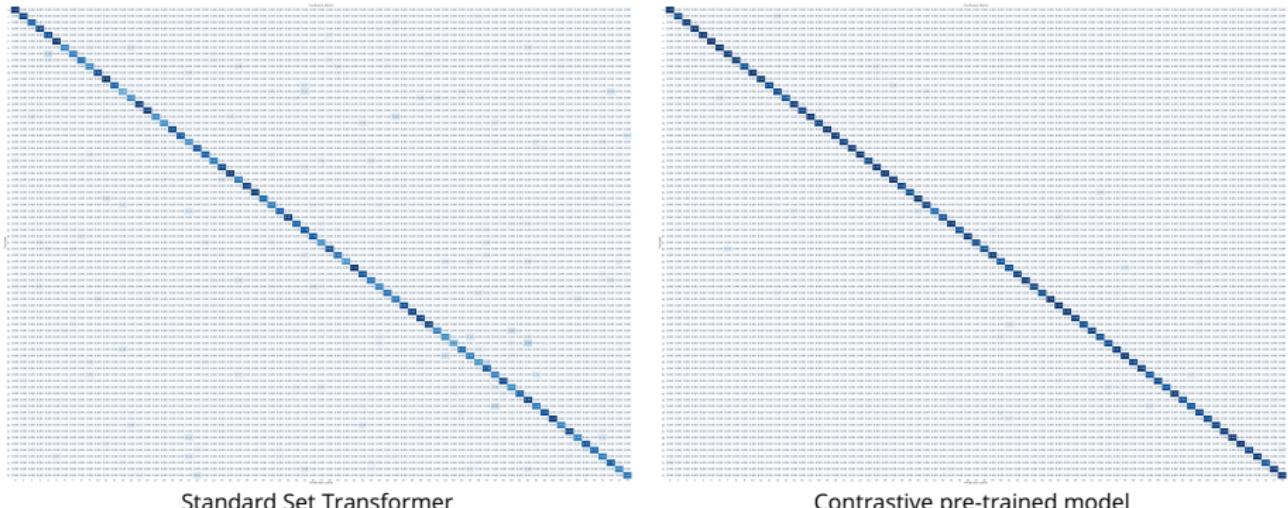


Figure 8: Weak Generalization averaged across Monte Carlo simulation

Table 1: Average accuracy results for Weak Generalization

Method	Average accuracy
Standard Set Transformer	87.6%
Contrastive Pre-trained model	96.93%



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Strong Generalization

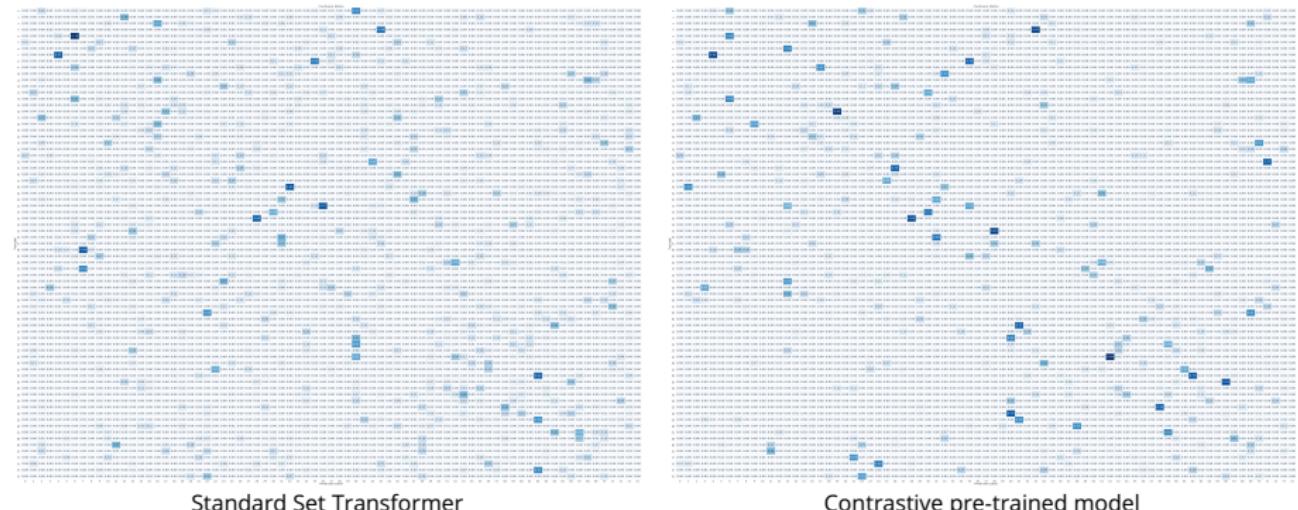


Figure 9: Strong Generalization averaged across Monte Carlo simulation

Table 2: Results for Generalization using KL Divergence

Method	KL Divergence
Standard Set Transformer	6.60
Contrastive Pre-trained model	6.25



Visualization

PCA Visualization for Standard Set Transformer



Figure 10: PCA Visualization for Standard Set Transformer

- Principal Component 1: 30.26%
- Principal Component 2: 24.38%
- Total Principal Component: 54.64%

Visualization

PCA Visualization for Contrastive Pre-trained Model

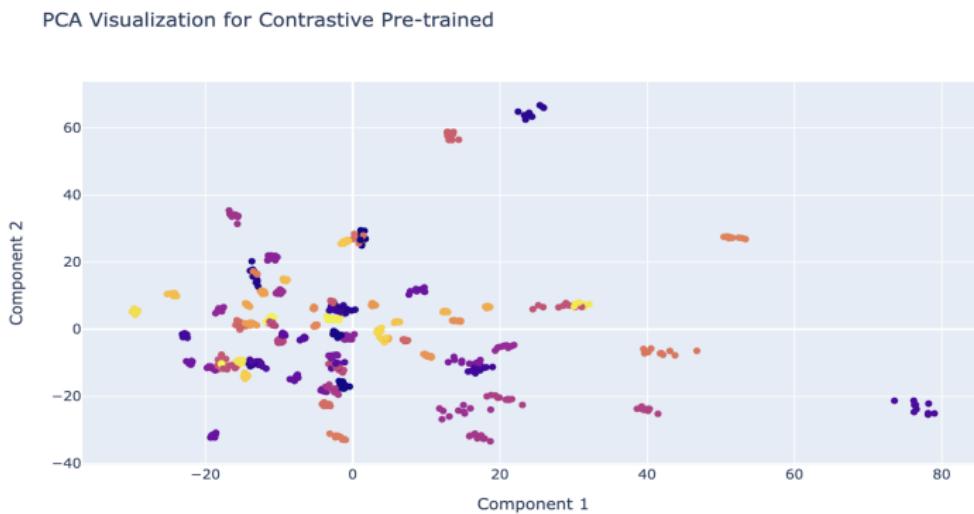


Figure 11: PCA Visualization for Contrastive Pre-trained

- Principal Component 1: 20.50%
- Principal Component 2: 18.35%
- Total Principal Component: 38.85%

Visualization

t-SNE Visualization for Standard Set Transformer

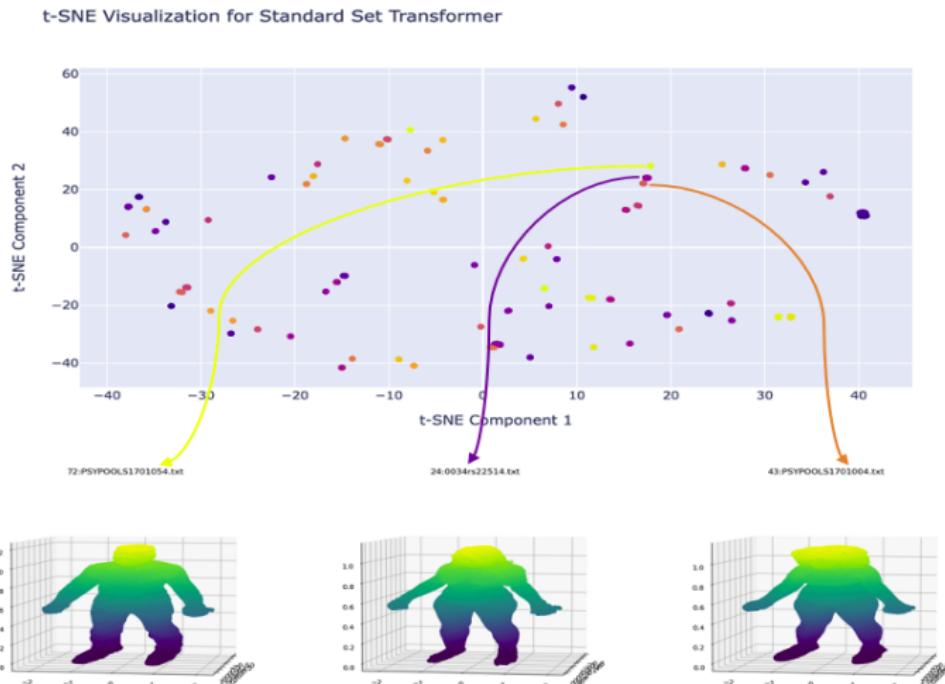


Figure 12: t-SNE Visualization for Standard Set Transformer



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Visualization

t-SNE Visualization for Standard Set Transformer

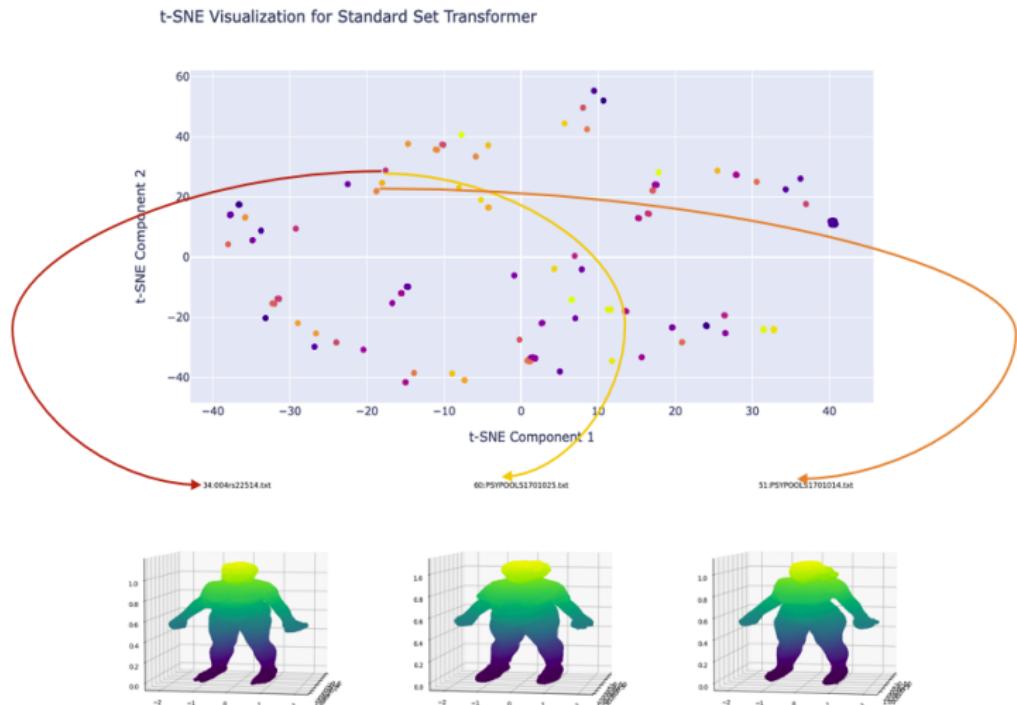


Figure 13: t-SNE Visualization for Standard Set Transformer



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Visualization

t-SNE Visualization for Contrastive Pre-trained Model

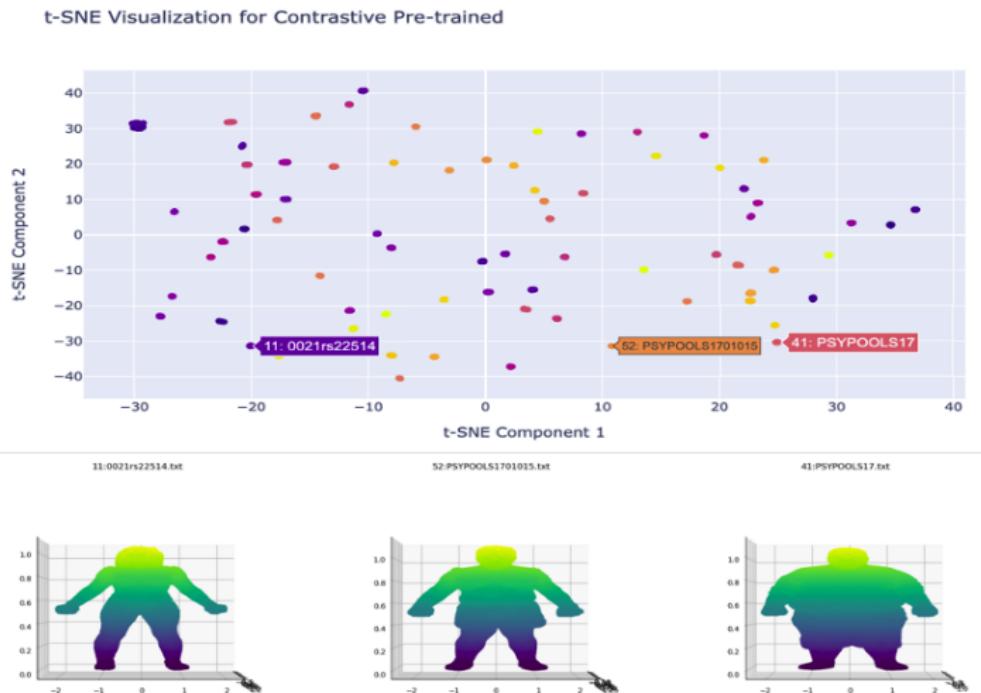


Figure 14: t-SNE Visualization for Contrastive Pre-trained Model



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Visualization

t-SNE Visualization for Contrastive Pre-trained Model

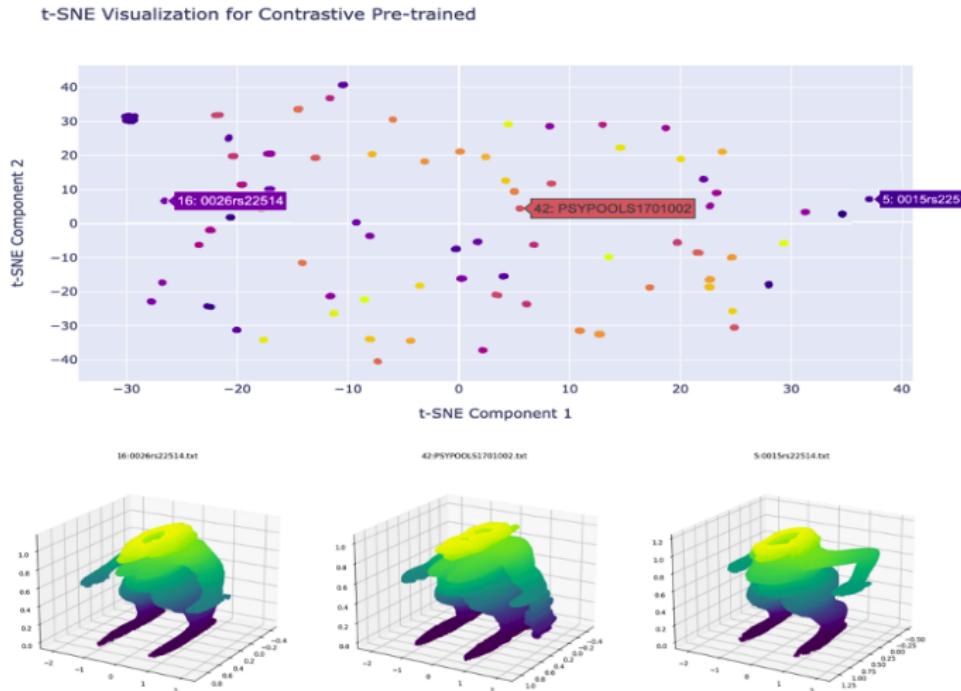


Figure 15: t-SNE Visualization for Contrastive Pre-trained Model



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Conclusion

- Standard Set transformer and Contrastive Pre-trained model for self-identification task.
- Weak and strong generalization for efficiency of the model.
- Contrastive Pre-trained model excelled Standard Set Transformer performance in terms of accuracy, speed, and stability.
- Contrastive pre-trained model showed improved generalization than the standard Set Transformer.



Conclusion

Future work

- Contrastive Pre-trained model can be used as a solid foundation for extended work like Generative Adversarial Set Transformer(GAST).
- GAST approach is to generate point cloud data to form a full or a partial 3D body scan.
- This approach is in the notion to provide support in case of missing scanned parts or lesser point cloud data that helps with increased precision.



Reference

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Thank you