Successful Contrastive Pretraining of Set Transformer

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Presentation Overview

Introduction

- Transformer - Process sequence of data
- Vision Transformer - Process images
- Set Transformer - Process unordered sets
- Contrastive Learning
- Generalization
  - Weak generalization
  - Strong generalization
- Point cloud 3D Body scan

Computational Science

Data

- 75 Participants
- Collected by Dr. Frederick Steven Cottle
- KX-16 Body Scanner [1]
- Point cloud count - 51000 to 63000

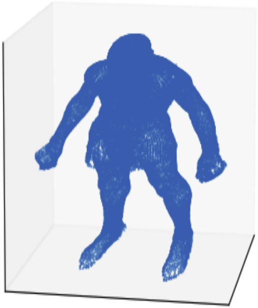


Figure: Original 3D Body Scan

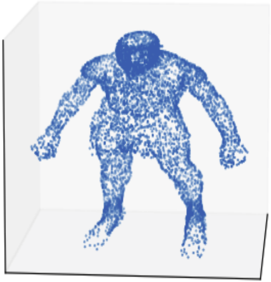


Figure: Subsampled 3D Body Scan

Background

- Set Transformer - Lee, J. et. al. (2018) [2]
  - Induced Set Attention Block(ISAB) - speeds up computation and extracts meaningful features.
  - Pooling layer - parameterized aggregation function, helps to capture the varying contribution of the instances, for better aggregation.

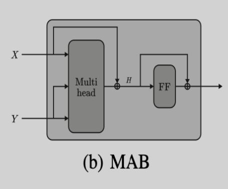


Figure: Multi Head Attention Block(MAB)[2]

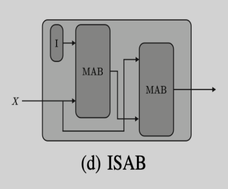


Figure: Induced Set Attention Block(ISAB)[2]

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]

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

Methods

- 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
- Loss - Sparse categorical cross entropy

Set Transformer

- Hyperparameters
  - Embedded dimension - 32, 64
  - Number of heads - 4, 16, 32
  - Induce points - 32, 64,128
  - stack - 2 to 6
  - Dropout - 0.05, 0.2
  - Optimizer - Adam
  - Learning rate - 1e-02 to 1e-04
  - Number of epochs - 250

Set Transformer

Set Transformer architecture

$y = Linear(3, embed\_dim)$
for $j = 1$ to $stack$ **do**
    $y = InducedSetAttentionBlock(y)$
end for
$y = Dropout(0.05)(y)$
$y = PoolingByMultiHeadAttention(y)$
$y_e mbedding = Droput(0.05)(y)$
$y = FinalDense(numberofclasses)(y\_embedding)$
$return\ y, y\_embedding$

Contrastive Learning using Set Transformer

- Base model - Set Transformer, to extract the feature embeddings
- For every batch a sample with its augmented self is a positive pair.
- For every batch a sample with the rest of the sample is negative pair.
- Experimented batch size - 4, 16, 32
- Point cloud - 8000, 2048, 1024
- Temperature - 0.5, 1.0, 2.0
- Optimizer - Adam with learning rate 1e-03

Contrastive Learning using Set Transformer

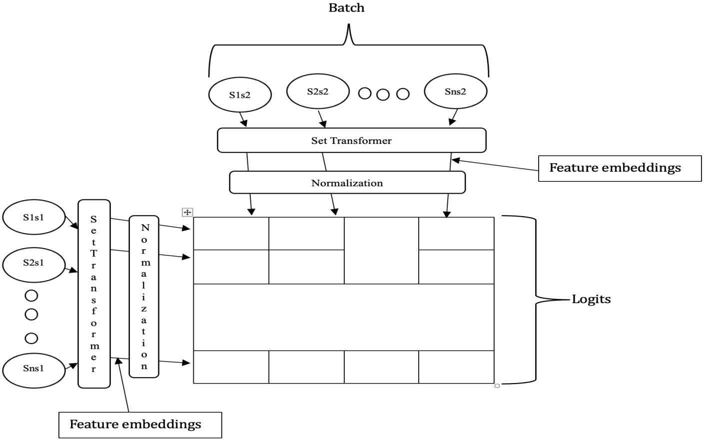


Figure: Contrastive Learning using Set Transformer architecture

Contrastive Learning using Set Transformer

Contrastive Learning architecture

1: $y1, y\_embedding1 = Set_Transformer(batch1)$
2: $y2, y\_embedding2 = Set_Transformer(batch2)$
3: $y\_embedding1 = Linear(embed\_dim, projection\_dim)(y\_embedding1)$
4: $y\_embedding2 = Linear(embed\_dim, projection\_dim)(y\_embedding2)$
5: $y\_embedding1 = Norm(y\_embedding1)$
6: $y\_embedding2 = Norm(y\_embedding2)$
7: $y = Mul(y\_embedding1, y\_embedding1.T) * Temperature$

Fine Tuning

- Additional Layers:
  - Linear layer - 1024, 256, 128
  - Non-linear activation function - LeakyReLU
  - Dropout - 0.1
- Hyperparameters - same as that of standard Set transformer

Generalization

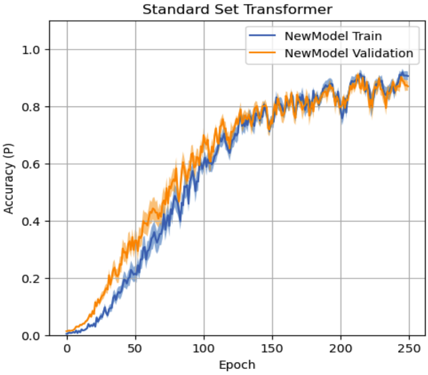
- Weak Generalization - Has knowledge about all the category data at the time of training.
- Strong Generalization(leave one out) - Is not aware of a particular class data at a given training period.
- Probability matrix - 75*75
- Reassign all diagonal elements in weak generalization 0.
- Normalize both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

Visualization

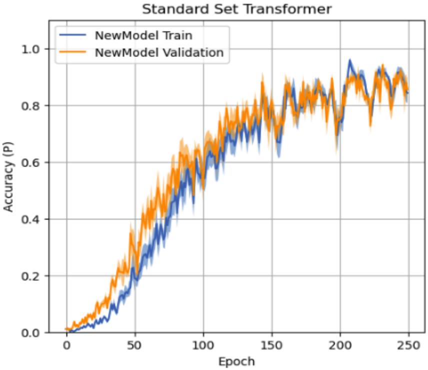
- Get feature embeddings for both standard Set transformer and Contrastive pre-trained model.
- 10 vectors for each sample.
- Applied PCA with 2 principal components to visualize in 2D.
- Applied t-SNE with a 2D component with the perplexity of 20.
- Evaluate along the 2D axis if, distribution is relatable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

Results

Standard Set Transformer



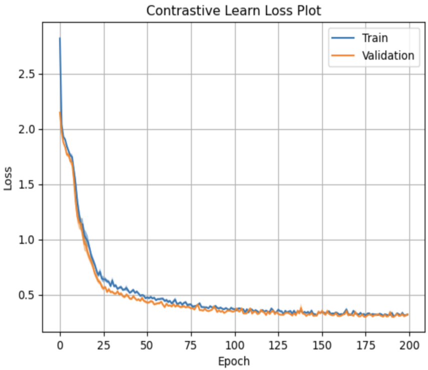
Good Result: 64,16,128,3,0.05



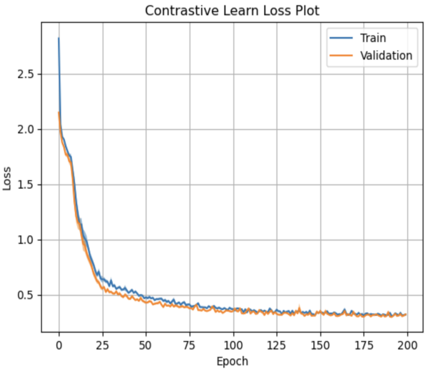
Bad Result: 64,32,128,3,0.05

Figure: Monte Carlo simulated Standard Set Transformer Accuracy

Contrastive Learning using Set Transformer



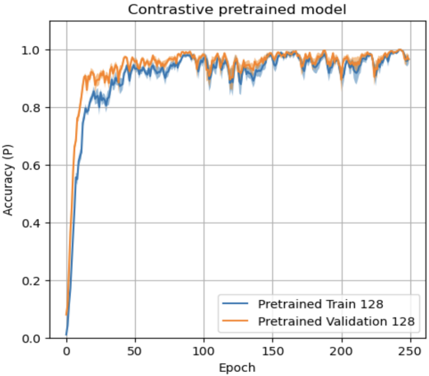
Good Result: 64,16,128,3,0.05



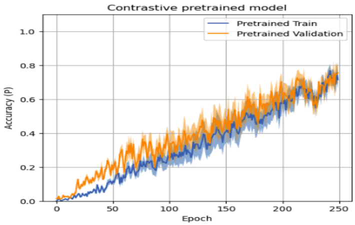
Bad Result: 64,16,128,3,0.05,batch size: 4

Figure: Monte Carlo simulated Contrastive Learning using Set Transformer Loss

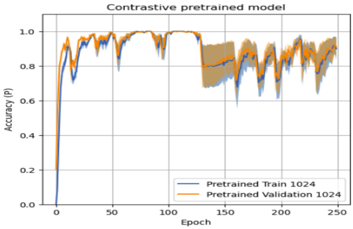
Fine Tuning



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



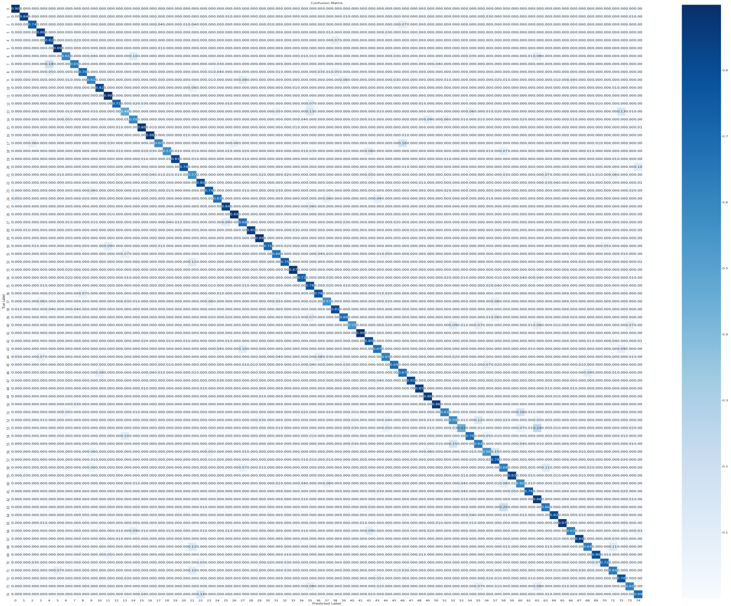
Bad Result: 64,32,128,3,0.05, 128, 0.1



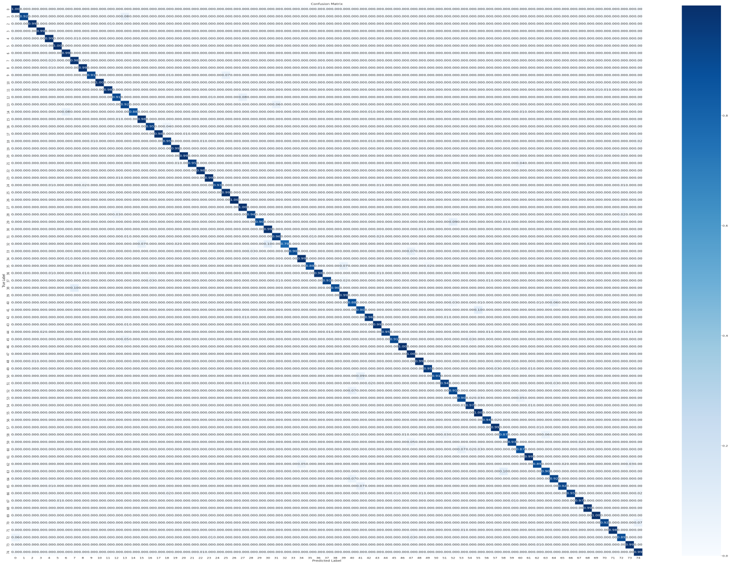
Bad Result: 64,16,128,3,0.05, 1024, 0.1

Figure: Monte Carlo simulated Contrastive pre-trained model Accuracy

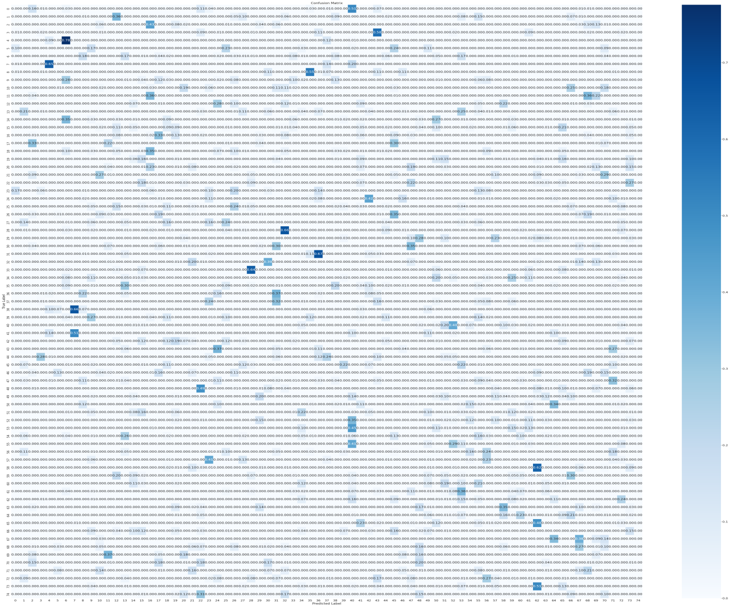
Weak Generalization: Standard Set Transformer



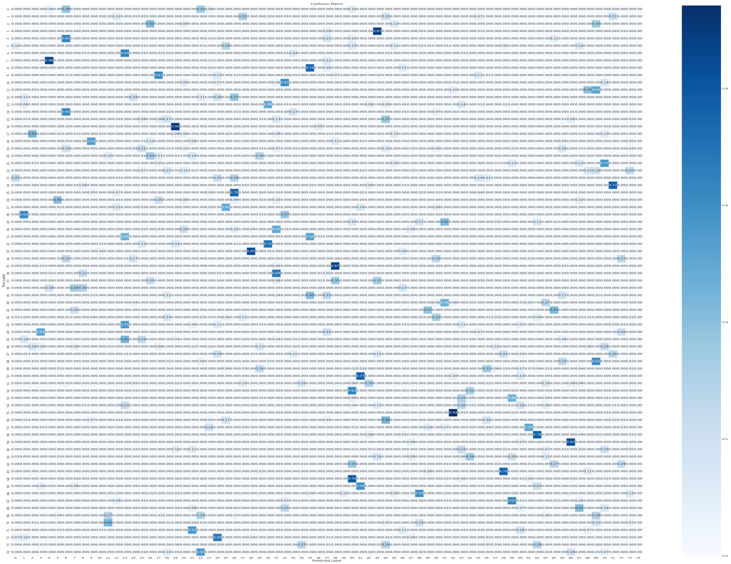
Weak Generalization: Contrastive pre-trained model



Strong Generalization: Standard Set Transformer



Strong Generalization: Contrastive pre-trained model



Generalization

Table: 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

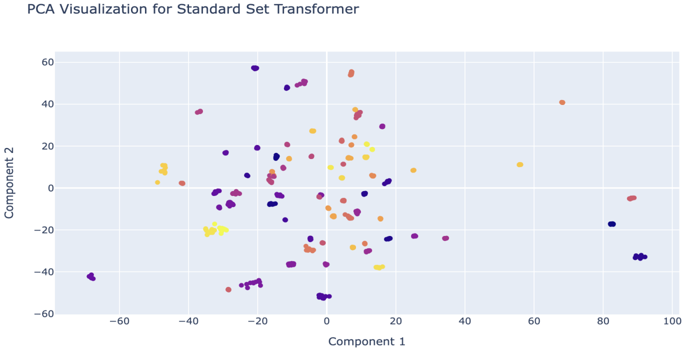


Figure: PCA Visualization for Standard Set Transformer

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

Visualization

PCA Visualization for Contrastive Pre-trained Model

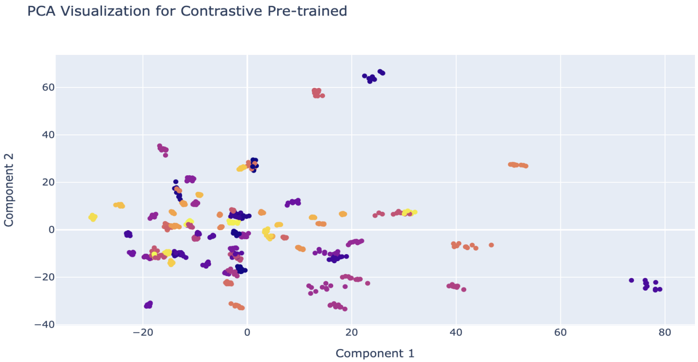


Figure: PCA Visualization for Contrastive Pre-trained

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

Visualization

t-SNE Visualization for Standard Set Transformer

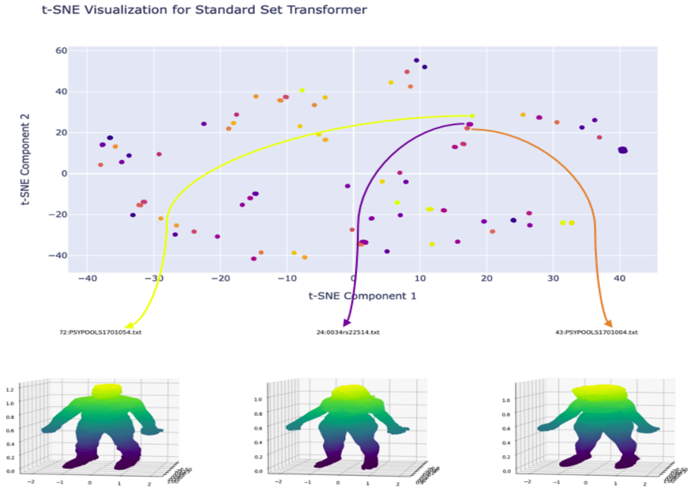


Figure: t-SNE Visualization for Standard Set Transformer

Visualization

t-SNE Visualization for Standard Set Transformer

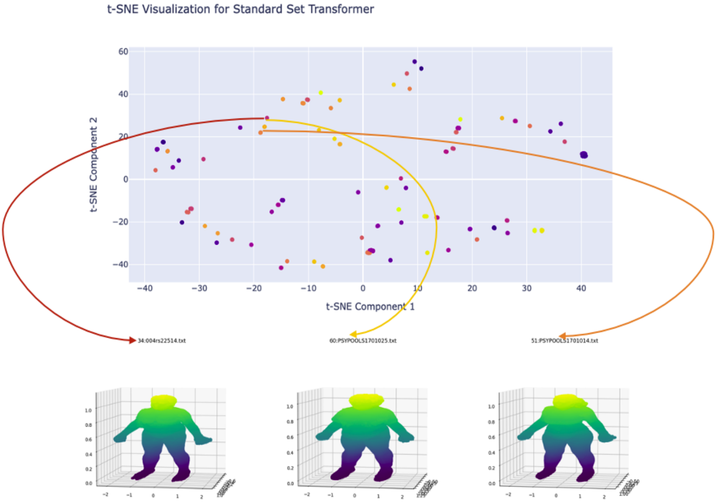


Figure: t-SNE Visualization for Standard Set Transformer

Visualization

t-SNE Visualization for Contrastive Pre-trained Model

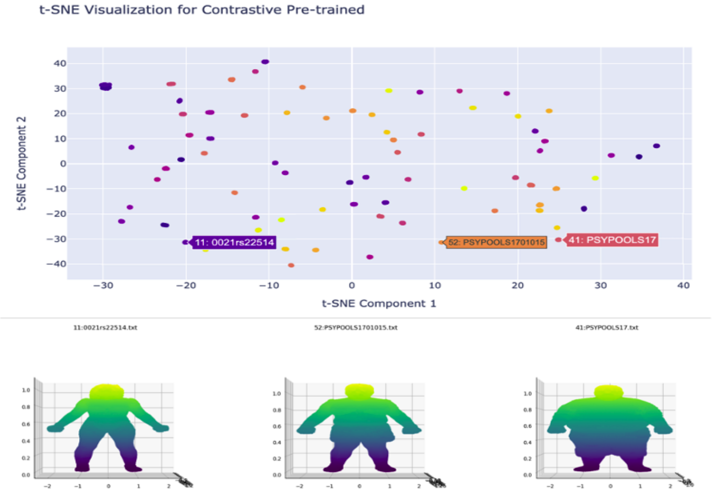
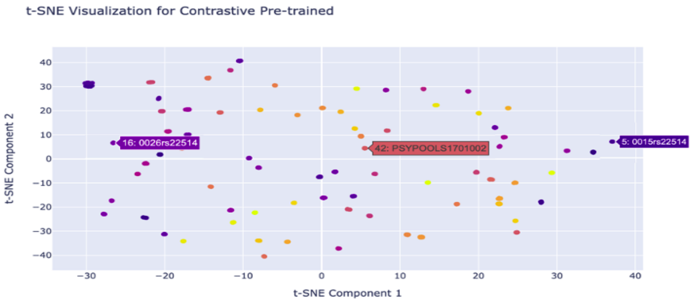


Figure: t-SNE Visualization for Contrastive Pre-trained Model



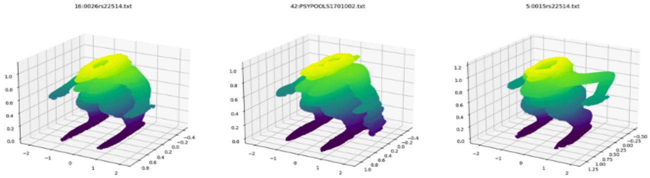


Figure: t-SNE Visualization for Contrastive Pre-trained Model

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.

- 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