

Final-year internship report

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## 3D Similarity for CAD Designs

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## Contents

1	Intr	oduction	1
In	$\operatorname{trod}_{}^{i}$	uction	1
	1.1	D3S, a leader in 3D CAD Analytics	1
	1.2	3D similarity model	2
2	Rela	ated work	5
	2.1	3D Understanding	5
	2.2	Contrastive learning	6
3	Met	chod	7
	3.1	Labeling application	7
	3.2	Triplet loss training	9
	3.3	Triplets generation	11
4 Ex		periments	13
	4.1	Training setups	13
		4.1.1 Data	13
		4.1.2 Triplets metrics	16
	4.2	Graph-based models	17
	4.3	Transformer-based models	19
	4.4	Visualizations	21
$\mathbf{C}^{\prime}$	anclu	sion	23

ii		$\mathbf{C}$	ontents
•	•		

5	5 Applications and perspectives			
Aı	pplica	ations	and perspectives	25
	5.1	Applie	cations	25
	5.2	Future	e Perspectives	25
	.1	Triple	ts generation heuristics	27
		.1.1	Triplets selection	27
		.1.2	Triplets filtering	28

# List of Figures

1.1	D3S, Data Science Softwares & Services	1
1.2	Purpose of our similarity model	2
1.3	Pipeline for building the model	3
3.1	User interface for the labeling use case. Here, the design on the right is more similar to the anchor design in the center (curved edges)	8
3.2	Two designs where the appropriate view is different	8
3.3	User interface for the validation use case. Here, the proposition of the model on the left is more similar to the anchor design in the center (two holes at the top)	8
3.4	The three types of negatives, given an anchor and a positive	10
4.1	Illustration of the issue using PCA as a preprocessing step. Both designs are tubular structures, shown in their default orientation and in the canonical reference frame. While the design on the left aligns its first principal axis with the tube's axis, the design on the right does not. This inconsistency can result in misalignment during training, particularly since the behavior varies depending on the specific design	14
4.2	Influence of the number of rotations on the rotations metrics	15
4.3	Influence of the type of data augmentation on the rotations metrics	16
4.4	GNN model key metrics accuracies	19
4.5	Fine-tuned model key metrics accuracies	20
4.6	Fine-tuned model rotation accuracies	20
4.7	t-SNE clustering of spherified sample embeddings	21
4.8	PCA clustering of spherified sample embeddings	22

ivList of Figures

Triplet selection process. An "anchor" point is selected, and a "positive" 1 point is found at a fixed target distance. A "negative" point is then found at a distance defined by the target distance plus a delta percentage. How far is the negative point matters a lot. If negative 1 is chosen, the triplet will likely be easy to label, but will not bring a lot of value to the model. If negative 2 is chosen, the triplet will likely be hard to label (and thus 

27

## Chapter 1

## Introduction

### 1.1 D3S, a leader in 3D CAD Analytics

D3S, which stands for Data Science Softwares & Services, specializes in delivering customized software solutions utilizing AI technologies. The company comprises a team of Data Scientists and Full Stack Developers with deep expertise in 3D CAD (Computer-Aided Design) Analytics and Natural Language Processing (NLP).

Its state-of-the-art technologies are built on open-source libraries and supported by internal R&D, enabling efficient data extraction through computer vision, Optical Character Recognition (OCR), and NLP. D3S also excels in deep learning applications such as 3D morpho analysis, metrics comparison, BoM (Bill of Materials) analytics, and time series processing.

The company's solutions are designed to provide scalable, adaptable, and secure business value for industries like aerospace and automotive.

I have been working with the 3D CAD Analytics team, where my focus was on developing a 3D similarity model designed to compare CAD designs solely based on their geometric properties.



Figure 1.1: D3S, Data Science Softwares & Services

2 Introduction

### 1.2 3D similarity model

3D design designers spend a significant amount of time searching for relevant information during the product design process, even though much of their work could be done by modifying existing Computer-Aided Design (CAD) designs. As a result, the retrieval and reuse of CAD designs are crucial in CAD design management. However, large CAD design repositories often require extensive categorization or organization of engineering data, making design reuse challenging. Traditionally, the classification and retrieval of 3D CAD designs involved a manual process of labeling, which is time-consuming, prone to errors, and inefficient. This issue becomes even more pronounced when designs are generated in product development, as inconsistent labeling and tagging across different systems lead to the complex task of data harmonization. Additionally, the inherent complexity of 3D CAD design definitions makes it difficult to apply rigid, general classification rules, as design features and parameters vary depending on their origin. Therefore, an automated approach to classification and retrieval is needed to address these challenges.

The goal is to automatically associate a given design to similar other designs, as depicted in Figure 1.2. This will make it possible to leverage the D3S dataset of industrial 3D designs, in order to infer missing information, such as the name of a design, its function, or its material.

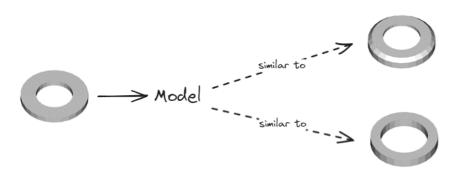


Figure 1.2: Purpose of our similarity model

In recent years, point cloud representations has become one of the research hotspots in the field of computer vision [25]. In our case, we can not directly train a powerful classifier, because of a lack of clean labeled data and of the variety of the possible 3D designs. Our most comprehensive labeled dataset available consists of just 2,000 CAD designs, with rather imprecise labeling. Examples of labels include coupling strap, shackle, and long beam. It is evident that there is a significant need for a more curated and accurate dataset in this area, which is really hard to obtain.

Given the recent success of self-supervised learning methods, more specifically contrastive learning [16, 24, 10], an innovative and promising approach has been proposed to tackle this problem.

The goal is to learn a representation of data such that similar instances are close together in the representation space, while dissimilar instances are far apart. To do so, a triplet loss, popularized by the FaceNet model [17], will be used. Since we lack labeled data, we can't generate triplets directly as in [17]. Instead, a 'Tinder-like' application has been developed and used by the whole company to build our labeled triplets database.

To clarify, a labeled triplet consists of three 3D designs: an anchor, a positive, and a negative design. The detailed framework of our triplet loss is outlined in section 3.2. In this setup, the anchor and positive designs are similar to each other, whereas the negative design is distinct from the anchor.

To summarize, the pipeline comprises the two main following steps:

- 1. **Triplets collection**: Offline unlabeled triplets are generated. Triplets are then labeled by the users of the app and stored in the database.
- 2. **Model training**: An encoding model is trained on the labeled triplets. The model is then used to compute the similarity between two 3D designs.



Figure 1.3: Pipeline for building the model

## Chapter 2

## Related work

### 2.1 3D Understanding

3D data can be presented in various formats, and the selection of the format is critical and depends on the specific needs of the application. A CAD design is a 3D representation of a physical object. At a higher level, the Standard for the Exchange of Product model data (STEP format) is a widely adopted ISO standard for data exchange that can represent 3D objects in CAD and related information. In this format, a CAD design is defined by its topological components such as faces, edges, or vertices and the connections between them. At a lower level, the STL format is a file format that represents 3D objects as a collection of triangles (mesh). This format is commonly used in 3D printing and computer graphics. Additionally, the point cloud format consists of a set of points in a 3D space, with each point representing a single point on the surface of the object. This format can be easily derived from an STL file by sampling points on the mesh surface. Other formats worth mentioning include voxel and multi-view image formats [25].

The decision was made to explore both STL and point cloud formats. The choice of the STL format is driven by its widespread use in the industry and the ease of generating a point cloud from it. Notably, designs based on the STEP format [11], while promising, were not considered because they limit the scope too much.

Following recent trends in the field, two main classes of models were investigated, graph-based models and transformer-based models.

#### Graph-based models

Graph neural networks (GNN) have been used recently in numerous applications [23, 9]. The flexible nature of a graph permits its usage from data sets concerning large social networks to smaller networks that describe the chemical bonds of a molecule. Graph neural

networks use the correspondences between elements instead of focusing on individual elements. These correspondences help create neighborhoods and local regions, which greatly enhance the predictive accuracy of the resulting features.

Given an input mesh, a natural candidate is a graph which nodes are the vertices of the mesh and where each vertex is connected to the vertices that share a face with it. This information is not available for the different GNNs that have been developed for 3D point cloud data [20, 21, 4]. These models are designed to work with point clouds. The main challenge is to define a graph structure that captures the local and global features of the point cloud. The most common approach is to define a graph where each point is a node and the edges are defined by the k-nearest neighbors of each point. The graph is then fed to a GNN to extract features from the point cloud.

#### Transformer-based models

Transformers [19] and self-attention models have revolutionized machine translation and natural language processing. They can equal or even surpass convolutional networks when applied to sequences and 2D images [5].

Self-attention is especially relevant in our context, as it naturally functions as a set operator, where positional information is treated as an attribute of elements within a set. Given that 3D point clouds consist of sets of points with positional attributes, the self-attention mechanism appears particularly well-suited to handling this type of data. Many recent works have explored the application of transformers to 3D data [26, 24, 10].

## 2.2 Contrastive learning

The goal of contrastive representation learning is to learn an embedding space in which similar sample pairs stay close to each other while dissimilar ones are far apart. Contrastive learning can be applied to both supervised and unsupervised settings. When working with unsupervised data, contrastive learning is one of the most powerful approaches in self-supervised learning [22].

Triplet loss is a widely used loss function in contrastive learning, made famous by the FaceNet model [17]. Numerous strategies have been suggested to enhance or refine the standard triplet loss [7, 6, 18]. Our approach incorporates some of these optimizations while leveraging our in-house labeling tool (section 3.1).

## Chapter 3

## Method

We propose a method for constructing a similarity model from an unlabeled dataset that contains a small proportion of approximately labeled instances. This method is applied on our use case of 3D CAD designs, but it is actually generalizable to other domains.

Unlabeled triplets are generated from the entire dataset section 3.3. These triplets are then labeled using a dedicated application section 3.1. Finally, the labeled triplets are used to train a model based on triplet loss section 3.2.

### 3.1 Labeling application

Before delving into the details of the pipeline, it is essential to introduce the user interface that has been developed in order to build the labeled triplets database.

There are actually two main use cases for the application: labeling triplets (Figure 3.1) and comparing two iterations of a model (Figure 3.3).

• Labeling triplets: Users are presented with a triplet of 3D designs, with the reference design (anchor) in the center. Their task is to swipe left or right to indicate whether the left or right design is more similar to the anchor design. A skip option is also available for ambiguous cases.

Users can also change to a canonical view of the designs to facilitate the comparison. This changes the perspective of a camera to a view aligned with the design's principal axes. This may or may not be useful depending on the design's geometry, as shown in Figure 3.2.

Additional metadata is also provided to the users, such as the design length. This information can help users make more informed decisions when the geometry does not suffice.



Figure 3.1: User interface for the labeling use case. Here, the design on the right is more similar to the anchor design in the center (curved edges).

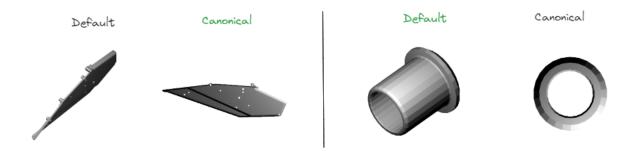


Figure 3.2: Two designs where the appropriate view is different.

• Validation: A similar interface is used, but now the propositions on the left and right are two nearest neighbors propositions of two different designs. Users judge which model gives the best nearest neighbor proposition. This gives an easy way to compare two iterations of a model. This is especially useful to bulletproof the model's performance, ensuring robustness not only in quantitative metrics but also in qualitative assessments.

This application is designed to be intuitive and user-friendly, allowing users to quickly and efficiently label triplets.



Figure 3.3: User interface for the validation use case. Here, the proposition of the model on the left is more similar to the anchor design in the center (two holes at the top).

Additional gamification elements were considered at one point, but they were deemed unnecessary as we were already achieving strong results with a small number of triplets.

### 3.2 Triplet loss training

The goal is to learn a representation of data such that similar instances are close together in the representation space, while dissimilar instances are far apart. We are going to use a triplet loss approach to train our encoder model. Once we will have our embeddings, the **cosine similarity** will be used to define a distance among the data points.

$$d(x,y) = 1 - \frac{x \cdot y}{\|x\| \|y\|}$$

The loss will be defined over triplets of embeddings:

- An anchor.
- A positive, of the same class as the anchor.
- A negative, of a different class than the anchor.

Given a batch size N, a distance function d, a margin margin and a, p and n tensors representing anchor, positive and negative examples, respectively.

$$\ell(a, p, n) = L = \{l_1, \dots, l_N\}^{\top}, \quad l_i = \max\{d(a_i, p_i) - d(a_i, n_i) + \text{ margin }, 0\}$$

Input tensors a, p and n are of shape (N, D), where D is the embedding dimension. The loss  $l_i$  is computed for each triplet in the batch, and the final loss is the mean of all individual losses.

Intuitively, you aim to group the data into separate clusters, ensuring that each class forms its own cluster. However, the precise distance between clusters isn't a concern, as long as they remain clearly distinct. Without limiting the loss, the model could improve by pushing an easy negative example very far away, while neglecting more challenging negative examples. By capping the reward beyond a certain distance, the model is encouraged to focus on the harder examples to continue improving.

Based on the definition of the loss, there are three categories of triplets:

- Easy triplets: Triplets which have a loss of 0, because d(a, p) + margin < d(a, n).
- Hard triplets: Triplets where the negative is closer to the anchor than the positive, i.e. d(a, n) < d(a, p).

• Semi-hard triplets: Triplets where the negative is not closer to the anchor than the positive, but which still have positive loss: d(a, p) < d(a, n) < d(a, p) + margin.

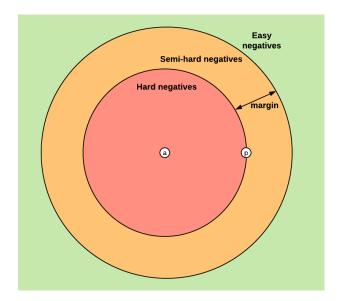


Figure 3.4: The three types of negatives, given an anchor and a positive.

The balance of these triplet types is crucial for the model's performance, as we will see in section 4.2.

Before delving deeper into working on triplet loss, we had to first ensure that training a triplet loss model with 'fake triplets' generated from our labeled dataset yielded similar results to a classification model trained on the same dataset. To do so, a GNN based on the EdgeConv architecure [21] was used.

The performance of the classification model was evaluated against the triplet loss model using a nearest neighbor approach. This method assessed how often a design's label matched that of its closest neighbor in the learned representation space. Both models achieved a 95% accuracy rate, suggesting that the triplet loss model successfully learned to create meaningful representations of the data. It is important to emphasize that at this point only triplets generated from the labels were used, and no human labeling was done. Triplets are generated following the same approach as in section .1, but ensuring that the anchor and the positive are indeed of the same class.

With just 1000 triplets, the model achieved a nearest neighbor accuracy similar to the classification model. However, optimal performance was observed when using approximately 10000 triplets, which resulted in a 95% accuracy rate.

### 3.3 Triplets generation

There is still the question of how to generate the triplets that are going to be labeled by the user of the app. Let's draw the properties of the triplets we want to generate, ordered by ease of implementation:

- 1. The triplets should be diverse enough to cover the entire dataset.
- 2. Almost every triplet should be 'labelable'. A triplet is 'labelable' if users do not have to skip it. This is a mainly a user experience concern.
- 3. A great proportion of triplets should be 'hard triplets' for the model that generated them, ie triplets where the negative is hard. This will force the next iteration of the model to learn from its misconceptions.

A simple yet effective way has been proposed to generate triplets. For the initial generation, a model trained on the small labeled dataset we had was used to compute embeddings for the entire dataset. This model was used to generate triplets based on heuristics which are detailed in section .1. Subsequently, the model was retrained on the labeled triplets, and the process was repeated iteratively.

With such a method, property 1 is straightforward to achieve, as a random selection of triplets will cover the entire dataset. Property 2 and 3 are in conflict, as a triplet that is easy to label is likely to be easy for the model as well. Considering the limits, selecting candidates that are equidistant from the anchor is intriguing, but tends to result in many 'skipped' triplets. Conversely, choosing candidates where the first is closer than the second will lead to fewer skipped triplets, but also a lower proportion of semi-hard and hard triplets.

It's why a proper balance has to be found, as explained in section .1.

## Chapter 4

## **Experiments**

Our final dataset for training the triplet loss model consisted of 20000 triplets, gradually accumulated through our labeling application. We employed consistent training configurations (section 4.1). The experiments were conducted using two different model architectures: GNN (item 4.2) and Transformer-based models (section 4.3).

### 4.1 Training setups

#### 4.1.1 Data

The dataset used for training the models consists of 20000 triplets, each containing three 3D designs: an anchor, a positive, and a negative model. Input data are meshes stored in stl files.

For the GNN model, vertices of the mesh are represented as nodes in a graph, while edges are defined based on the connectivity of the vertices. When two vertices share a face, an edge is created between them. For the transformer model, that take as input a point cloud, we convert the mesh into a point cloud by sampling points uniformly from the surface of the mesh. The number of sampled points is fixed to 10000, following [10].

Initially, the use of Principal Component Analysis (PCA) for training or inference, as done in [13], was considered but ultimately discarded. The idea of PCA is appealing because it allows working within a canonical reference frame. However, to ensure the model is as general as possible, data augmentation techniques were favored over PCA. One of the issues with PCA is demonstrated in Figure 4.1. Additionally, we prefer to let the model architecture handle these aspects directly.

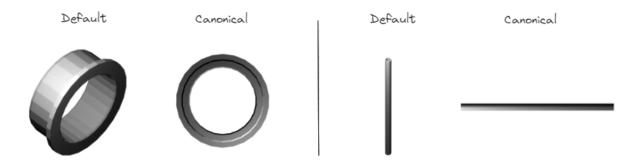


Figure 4.1: Illustration of the issue using PCA as a preprocessing step. Both designs are tubular structures, shown in their default orientation and in the canonical reference frame. While the design on the left aligns its first principal axis with the tube's axis, the design on the right does not. This inconsistency can result in misalignment during training, particularly since the behavior varies depending on the specific design.

Data augmentation was performed to enhance the model's robustness, especially considering rotations. Other augmentation techniques, such as symmetry and noise addition, were also explored but ultimately discarded. The following two techniques were retained:

- 1. **Normalization to unit sphere**: We standardize all the designs to fit within a unit sphere. This enhances the model's ability to capture geometric features rather than scale. The length of the design has been integrated into the architecture of the GNN model.
- 2. Random rotations: Each design is randomly rotated around the three axes. This is crucial for ensuring that the model learns to recognize designs regardless of their orientation. A special focus was placed on rotation invariance, as explained hereafter.

Rotation invariance is a critical aspect of our model, as it allows the model to recognize designs regardless of their orientation. This is particularly important in our context since 3D designs designers often work with similar designs saved in different orientations. To achieve this, 3 metrics were defined to evaluate the model's performance in terms of rotation invariance:

- Mean distance to rotated distribution: This metric calculates the average distance between the model's prediction of a design and the predictions of its n rotated versions.
- Median distance to rotated distribution: Similar to the mean distance, this metric computes the median distance between the model's prediction and the predictions of the n rotated versions.

• Rotation matching accuracy: The two previous metrics are absolute. To provide a more relative measure, we also compute a rotation matching accuracy. If we fix a value of n, we can compute the proportion of nearest neighbors in the whole dataset that are also among the n rotated versions of the design. n is set to 10 in our experiments, as for the two previous metrics.

Initially, data augmentation was performed offline. This means that for each triplet, each design was augmented by applying random rotations before the training process. We choose 10 rotations per design, as it yields the best results as shown in Figure 4.2. Results are shown with our starting GNN EdgeConv model.

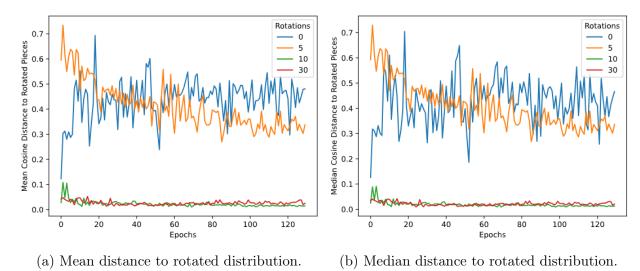
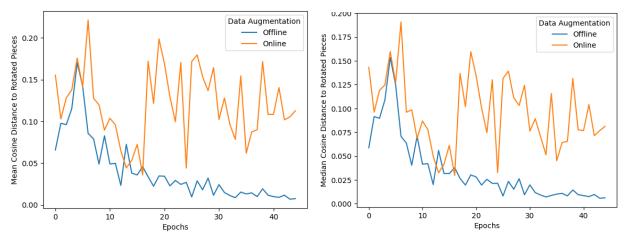


Figure 4.2: Influence of the number of rotations on the rotations metrics.

We also experienced online data augmentation, where random rotations are applied on-the-fly during training. Indeed, there is no clear recipe for the best approach [3] and we wanted to explore both options. The results of both approaches are compared in Figure 4.3. The offline augmentation approach yielded better results.



- (a) Mean distance to rotated distribution.
- (b) Median distance to rotated distribution.

Figure 4.3: Influence of the type of data augmentation on the rotations metrics.

#### 4.1.2 Triplets metrics

Training a triplet loss model is notoriously difficult. To better monitor the training process, several metrics were defined:

- Train easy triplets proportion: This metric computes the proportion of easy triplets in the training set. An easy triplet results in a loss of 0.
- Test easy triplets proportion: This metric computes the proportion of easy triplets in the test set.
- Training triplets order: This metrics computes the proportion of triplets that are 'correctly' ordered. A triplet is correctly ordered if the distance between the anchor and positive is less than the distance between the anchor and negative. This is the same as an easy triplet proportion for a triplet loss with margin 0.
- Original triplets order: This metrics computes the proportion of triplets that are 'correctly' ordered in the original dataset. It is important to notice here that these triplets do not belong to the training triplets, because the training triplets are augmented with random rotations.

Proportions of the training data were incorporated to analyze the model's behavior when converging to a loss of 0. The order of triplets was included to both assess the impact of the margin on triplet loss and to align with the fact that this order ultimately matters, as it's the one used by app users for labeling.

In addition to these metrics, we also computed the accuracy of the model on the small labeled dataset by evaluating the proportion of designs which nearest neighbor shares the same label. This metric is referred to as the **test accuracy**. We had to keep in mind that this accuracy gives a biased view of the model's performance, as the labeled dataset is not representative of the whole dataset.

We had also a heavy use of the interface to validate the model's performance qualitatively. Indeed better metrics do not always correlate with better real performance as it is shown in section 4.3.

### 4.2 Graph-based models

Our original architecture involved a GNN model based on EdgeConv [21] convolution layers along with max pooling layers.

Different convolution layers were tested for our backbone encoder, including Pointnet [14], FeaStConv [20], and PointTransformerConv [26]. The EdgeConv model was chosen as it yielded the best results.

On the one hand, EdgeConv operates on each node's local neighborhood, computing feature transformations for connected edges and aggregating this information. This captures local graph structure and node relationships.

The max pooling layer then aggregates information across all nodes, creating a fixed-size graph representation that is invariant to the number of nodes and their ordering. Given a graph with N nodes, F features and a feature matrix X (N rows, F columns), global max pooling pools this graph into a single node is just one step. To compute the feature vector of this pooled node, it takes the feature-wise maximum across the node dimension of the graph. In other words, global max pooling finds for each feature/column in X the node with the highest value and then takes this value into the pooled node vector.

This combination allows the model to learn both local and global graph features effectively. The model works well because it can capture complex relationships in graph data, is scalable to different graph sizes, and learns hierarchical representations through stacked layers.

Here are a few key learnings we gathered along the way:

Use batch normalization Batch normalization [8] turns out to be a crucial component for training our model. Not only does it speed up the training process, but it also improves the model's performance. This is particularly true for a similarity model, where the model must learn to differentiate between designs based on their cosine similarity. Dropout was also used in order to prevent overfitting.

Use large batch sizes Batching graph data is challenging because the number of nodes in each graph can vary. A dynamic batching strategy was implemented to handle this issue, fixing a maximum number of nodes per graph. The size of the batch has a real impact on the model's performance. A larger batch size allows the model to learn more effectively, as it allows a greater triplets diversity within a single batch. We particularly observed this significance due to a change in the mesher for company-related reasons. Indeed, switching from Gmsh [2] to BRepMesh\_IncrementalMesh [1] led to different mesh sizes and configurations. The meshes generated from the BRepMesh were more complex, which reduced inevitably the batch size during training. We experienced a drop in the model's performance, but still good results. This shows the relative flexibility of such a model to adapt to different mesh format. This experience motivated us to explore the use of point clouds methods, such as the transformer-based model. These are more flexible because a uniform sampling can be applied to any mesh.

Insights into the triplet loss Triplet loss is notoriously difficult to train. Both the distance function and the margin can have a significant impact on the model's performance. The euclidean distance, notably used in FaceNet [17], was tested but ultimately discarded in favor of the cosine similarity. The cosine similarity tends to be more robust to rotation changes, which is crucial for our model. The margin was set to 0.5, as it yielded the best results.

We soon encountered the problem of the loss rapidly converging to 0. It's why we added the triplets metrics introduced in subsection 4.1.2 to better monitor the training process. Despite the loss trending towards zero, the classification accuracy began to decline just a few epochs after reaching peak values. It became evident that many of the triplets were quickly classified as 'easy triplets' by the network. At this juncture, it was unclear whether the subsequent training performance was affected by the model architecture or the training loop itself.

To address the issue, in addition to adjusting the learning rates and dropout parameters, we implemented online triplets filtering within each batch, in order not to take into account certain type of triplets within the reduction. Indeed, the loss is rapidly converging to 0 because most of the elements within the reduction equal to 0.

In order of their performance:

- 1. **Hard** + **Semi-Hard triplets filtering**: This approach involves only keeping the hard and semi-hard triplets.
- 2. **Semi-Hard triplets filtering**: This approach involves only keeping the semi-hard triplets.
- 3. Hard triplets filtering: This approach involves only keeping the hard triplets.

Since we are working in an unsupervised setting, it is not possible to generate triplets on the fly, like is suggested in [12]. Also, triplets that are classified as easy triplets at a given epoch can't just be discarded from the training set, as they might become hard triplets at a later epoch.

As shown in Figure 4.4, the model quickly reaches a great accuracy on the test set. However, the original triplets order metrics starts decreasing after a few epochs, even if the loss continues to decrease. This shows the limitations of this architecture, as it is not able to further learn the correct order of the triplets. This tendency will be fixed by using a transformer-based model.

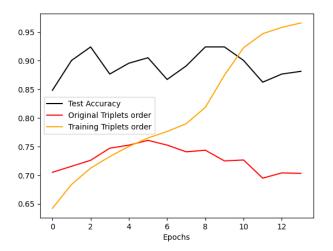


Figure 4.4: GNN model key metrics accuracies.

### 4.3 Transformer-based models

As explained previously, several points made us pivot towards point cloud transformer models.

- Growing popularity of point cloud transformer models in the field of 3D data processing.
- Flexibility of point cloud models. They are less dependent on the input mesh format, as a uniform sampling can be applied to any mesh.
- Easy switch from a mesh to a point cloud format.

The goal was to study the performance of a pre-trained encoding model our on data, as well as a fine-tuned model with our triplets. Several backbones were tested, such as Re-Con++ [15] or PointTransformer [26]. The best results were obtained with the OpenShape

model [10], which architecture is derived from PointBERT [24]. Indeed, the pre-trained model already showed improved performance in comparison with our best GNN model, as it can be seen from the starting performance in Figure 4.5. The fine-tuned model was able to reach even better results, as shown in Figure 4.5.

We can clearly see the increasing metrics as the loss decreases, which was clearly not the case with the GNN model. The model is able to learn the correct order of the triplets, as shown by the original triplets order metrics. The rotation metrics are also improving, as shown in Figure 4.6. This highlights the remarkable ability of transformers architectures to learn intricate patterns in the data, regardless of its nature.

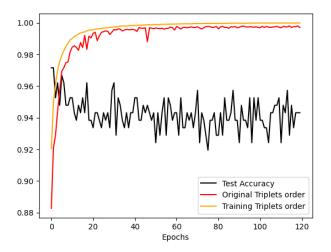


Figure 4.5: Fine-tuned model key metrics accuracies.

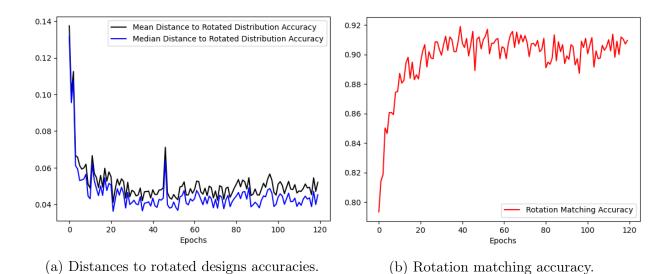


Figure 4.6: Fine-tuned model rotation accuracies.

4.4. Visualizations 21

### 4.4 Visualizations

As a final benchmark, we compared in the interface the nearest neighbors of a design given by the transformer pre-trained model and by the fine-tuned model. Even if fine-tuned model is better in terms of metrics, the qualitative results are not always better. This shows the limitations of the metrics and the importance of the interface to validate the final model's performance, especially in our unsupervised setting.

It's also interesting to visualize the embeddings in a 3D space. These show the model's ability to cluster similar designs together, even without explicit labels for the designs. The model is truly able to learn the underlying geometric features of the designs, as shown in Figure 4.8 and Figure 4.7.

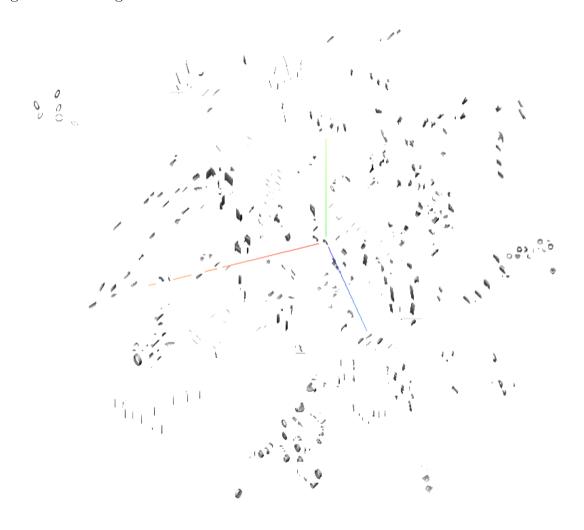


Figure 4.7: t-SNE clustering of spherified sample embeddings.

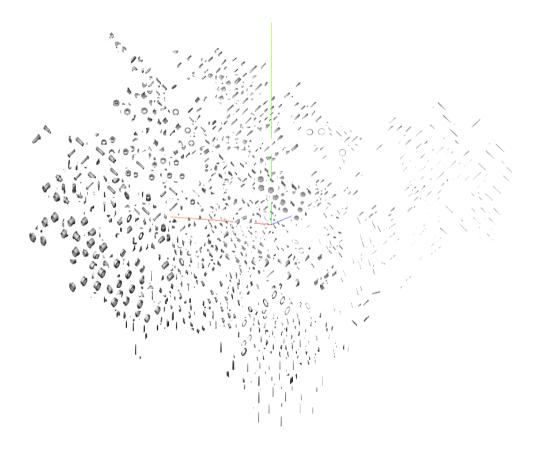


Figure 4.8: PCA clustering of spherified sample embeddings.

## Conclusion

This work presents a novel approach to addressing the challenge of 3D CAD design similarity in industrial settings, where large repositories of designs often lack consistent labeling and organization. We developed a pipeline that combines innovative triplet generation techniques, a user-friendly labeling application, and state-of-the-art deep learning models to create an effective similarity model for 3D CAD designs. Our key contributions include:

- A method for generating unlabeled triplets from an extensive dataset of 3D designs, balancing diversity, labelability, and difficulty.
- A "Tinder-like" application that facilitates efficient human labeling of triplets, incorporating both default and canonical views to aid in comparison.
- An iterative process of model training and triplet generation, allowing the model to continuously improve by learning from its previous misconceptions.
- Experimentation with both graph-based (GNN) and transformer-based models, ultimately finding superior performance with the transformer-based approach.

The experiments conducted demonstrate the effectiveness of our approach. The graph-based model using EdgeConv layers showed promising initial results, achieving high accuracy on the test set. However, it struggled to maintain performance on the original triplet order metric over extended training. The transition to a transformer-based model, specifically using the Openshape encoder architecture, yielded significantly improved results. This model not only maintained high performance across all metrics but also showed continuous improvement in triplet ordering and rotation invariance as training progressed.

One of the main advantages of our approach is its capacity to learn meaningful representations from a relatively small set of labeled triplets. With only 20,000 triplets, we successfully trained a GNN model that exceeded our initial expectations and demonstrated strong performance across multiple metrics, although it falls short of the larger transformer model. The pre-trained version already shows superior results, and fine-tuning further enhances its performance.

However, our work also has some limitations:

24 Conclusion

• The reliance on human labeling, while mitigated by our efficient application, still introduces a bottleneck in scaling to very large datasets.

• The potential for bias in the triplet generation process, which may not fully capture all nuances of design similarity.

In conclusion, this work represents a significant step forward in automating the classification and retrieval of 3D CAD designs. By leveraging human expertise through targeted labeling and state-of-the-art deep learning techniques, we have created a robust similarity model that can greatly enhance the efficiency of design reuse and information retrieval in industrial settings.

## Chapter 5

## Applications and perspectives

### 5.1 Applications

Immediate applications of the similarity model developed in this work include:

#### 1. Automated Design Optimization:

- Leveraging the similarity model to suggest design improvements based on highperforming similar designs.
- Developing generative models that can propose new designs based on similarity-driven interpolation between existing successful designs.

#### 2. Integration with CAD Software:

- Embedding the similarity model directly into CAD software for real-time suggestions during the design process.
- Creating plugins that allow for similarity-based search and retrieval directly within popular CAD environments.
- Embedding the model into D3S Costing Platform.

## 5.2 Future Perspectives

The work presented here opens up several avenues for future research and development:

#### 1. Multi-modal Similarity Models:

• Integrating geometric data with textual descriptions, functional specifications, or material properties to create more comprehensive similarity metrics.

• Exploring the use of large language models to bridge the gap between natural language queries and geometric design features. [10] uses CLIP to distill 2D and text representations knowledge to the 3D modality, but more recent papers like [15] use GPT 4 to chat with 3D models.

#### 2. Labeling tool for Active Learning:

• Implementing active learning strategies to intelligently select new triplets for labeling, maximizing the information gain from human input.

### .1 Triplets generation heuristics

#### .1.1 Triplets selection

For each anchor data point, we fix a target distance, and a delta percentage. We can in this way find a first data point which distance to the anchor data point is close to the fixed target distance.

Then, we can find a second data point which distance to the anchor data point is close to the fixed target distance **plus** a percentage of this target distance, defined by delta. We have to be careful not to propose the same data point here (especially working with small values).

The proposed triplet is the concatenation of these three data points. In the following, for simplicity, we will call these 3 data points respectively the anchor, the positive and the negative, even if the proposed negative can actually be the real positive (hard triplet).

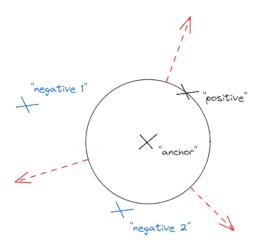


Figure 1: Triplet selection process. An "anchor" point is selected, and a "positive" point is found at a fixed target distance. A "negative" point is then found at a distance defined by the target distance plus a delta percentage. How far is the negative point matters a lot. If negative 1 is chosen, the triplet will likely be easy to label, but will not bring a lot of value to the model. If negative 2 is chosen, the triplet will likely be hard to label (and thus skipped), but will bring a lot of value to the model.

We initially used target distances uniformly distributed between 0.001 and 0.05, and delta uniformly distributed between 0.1 and 0.5.

These hyperparameters must be tuned according to the dataset. Iterative visual inspections were conducted to ensure that the triplets generated were relevant according to the properties defined in section 3.3.

#### .1.2 Triplets filtering

Once our triplets are selected, we have to filter some triplets that do not bring enough value, or that will be too hard for the user to label.

- 1. Concatenation of the triplets found for each pair of parameters can lead to duplicate triplets -> Duplicated triplets are discarded.
- 2. It turns out that triplets with the same anchor and positive points share really similar negative point -> Duplicated (anchor, positive) triplets are discarded.
- 3. Working with small target distances and deltas can lead to undesirable behaviours -> Triplets where the distance from the anchor to the positive 0 are discarded. Triplets where the distance from the anchor to the positive is greater than the distance from the anchor to the negative are discarded.
- 4. Sometimes, the positive and the negative data points turn out to be pretty similar -> Triplets where the relative distance from the positive to the negative is greater than a percentage of the distance from the anchor to the positive are discarded.

All these filters aim at reducing as much as possible the amount of triplets that won't be labeled by the user.

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