Similarity Learning and Data Generators

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Abstract

Similarity learning techniques can be a powerful tool for research and data analysis, however, the tools for supporting such methods are few and far between. This paper explores many different methods in which data generators may be developed for similarity learning algorithms, primarily focused on the Siamese Neural Network architecture.

Background

As a point of reference, this paper will be focusing on siamese neural networks and its respective data generators, however, this data paper may still hold value to other fields of research, void of any connection to siamese neural networks. This paper has utilized some common terms, idiomatic expressions, and lingo specific to both data generation and machine learning, which will be addressed now:

Table 1: *Common Terms and Definitions*

Term	Definition
AI/ML	Artificial Intelligence/Machine Learning
SiNN	Siamese Neural Network
Scrape	To aggregate information

What Is AI/ML?

AI was originally coined by John McCarthy in 1955, before being further defined as "the construction of computer programs that engage in tasks that are currently more satisfactorily performed by human beings because they require high-level mental processes such as: perceptual learning, memory organization and critical reasoning"[1, 2].

Now AI is a broad term used to describe just about any learning process being completed by a computer, however, in simplest terms it is a computer task that creates a function which is trained to predict outputs based on inputs.

A **batch** is a set of data that is used to train a neural network, where after each set of data the internal model parameters (in Neural Networks it would be weights and biases) are changed. A **batch size** is then the number of samples in each batch. The purpose of an **epoch** is then the number of times the model would make a full pass through the entire dataset [3]. Therefore, in an epoch, there may be multiple batches (or batch iterations), and subsequently multiple **gradient descent steps**.

However, in the case of dynamic generators (ones that don't necessarily represent the entire dataset and are generated dynamically) such as the one this paper, an **epoch** will describe the number of times a batch is passed to a model, because there will only be one batch iteration, and subsequently one **gradient descent step** per epoch.

overfitting and training

What Is Deep Learning?

Deep Learning is a more specific branch of AI that is typically associated with multi-layer neural networks (more than 3) also with the purpose of training values to better predict outputs dependent upon inputs.

What Is Similarity Learning?

Similarity is a very specific branch of ML that is used for determining the similarity between different data sets[4].

What Are Siamese Neural Networks?

A SiNN is a kind of similarity learning approach to comparing images (or other 2D data), and determining their similarity. SiNNs leverage one neural network which is used to classify each individual image, which can then be used to find the euclidean distance and the overall similarity of the images.

Table 2: *Tensorflow arguments for image_dataset_from_directory()*

Short	Long
directory	Directory where the data is located.If labels is "inferred", it should containsubdirectories, each containing images for a class.Otherwise, the directory structure is ignored.
labels	Either "inferred"(labels are generated from the directory structure),None (no labels),or a list/tuple of integer labels of the same size as the number ofimage files found in the directory. Labels should be sorted accordingto the alphanumeric order of the image file paths(obtained via os . walk(directory) in Python).
label _ mode	String describing the encoding of labels . Options are: 'int': means that the labels are encoded as integers(e.g. for sparse_categorical_crossentropy loss). 'categorical' means that the labels areencoded as a categorical vector(e.g. for categorical_crossentropy loss). 'binary' means that the labels (there can be only 2)are encoded as float32 scalars with values 0 or 1(e.g. for binary_crossentropy). None (no labels).
class _ names	Only valid if "labels" is "inferred". This is the explicitlist of class names (must match names of subdirectories). Usedto control the order of the classes(otherwise alphanumerical order is used).
color _ mode	One of "grayscale", "rgb", "rgba". Default: "rgb".Whether the images will be converted tohave 1, 3, or 4 channels.
batch _ size	Size of the batches of data. Default: 32.If None , the data will not be batched(the dataset will yield individual samples).
image _ size	Size to resize images to after they are read from disk,specified as (height , width) . Defaults to (256 , 256) .Since the pipeline processes batches of images that must all havethe same size, this must be provided.
shuffle	Whether to shuffle the data. Default: True.If set to False, sorts the data in alphanumeric order.
seed	Optional random seed for shuffling and transformations.
validation _ split	Optional float between 0 and 1,fraction of data to reserve for validation.
subset	Subset of the data to return.One of "training", "validation" or "both".Only used if validation _ split is set.When subset="both" , the utility returns a tuple of two datasets(the training and validation datasets respectively).
interpolation	String, the interpolation method used when resizing images.Defaults to bilinear . Supports bilinear , nearest , bicubic , area , lanczos3 , lanczos5 , gaussian , mitchellcubic .
follow _ links	Whether to visit subdirectories pointed to by symlinks.Defaults to False.
crop _ to _ aspect _ ratio	If True, resize the images without aspectratio distortion. When the original aspect ratio differs from the targetaspect ratio, the output image will be cropped so as to return thelargest possible window in the image (of size image _ size) that matchesthe target aspect ratio. By default (crop _ to _ aspect _ ratio=False),aspect ratio may not be preserved.
*kwargs	Legacy keyword arguments.

Introduction

Requirements of The Data Generator

Many libraries exist now for generating, changing, and augmenting data, however, there has been some amount of underdevelopment in the area of SiNNs, which can in large part be attributed to the lack of data generation or generation tools for such architecture. As the architecture requires data that is formatted in a manner that is different than most other kinds of AI/ML, especially kinds which are not under the umbrella of similarity learning.

The purpose of this paper is to expose possible methods of data generation for SiNNs, both as a stand alone generator (one that isn't dependent on other AI/ML

libraries), as well as one that may interface with the Tensorflow library.

Arguments / Inputs To The Generator

Regarding the development of the generator, this paper seeks to mimic the pre-existing tensorflow function “tf.keras.utils.image_dataset_from_directory”, and match the arguments (Table 2) that are supported by the aforementioned function[5] in the Tensorflow integration explained later on.
However, prior to this there will be a stand alone generator developed for the same purpose. The focus, however, of the standalone is to provide a more fundamental understanding of the generator and will use the following limited list of arguments:

- directory
- batch_size

Output Of The Generator

For the generator which this paper will contribute to Tensorflow, it will match as closely as possible to the already existing "image_dataset_from_directory". This existing function has an output which is dependant upon arguments which we will not be taking for the stand alone generator, and will thus be different in terms of output.

Table 3: *Output of image_dataset_from_directory*

A tf.data.Dataset object.
If label_mode is None, it yields float32 tensors of shape (batch_size, image_size[0], image_size[1], num_channels), encoding images (see below for rules regarding num_channels). Otherwise, it yields a tuple (images, labels), where images has shape (batch_size, image_size[0], image_size[1], num_channels), and labels follows the format described below.

The output of the stand alone generator will them be the following: (images, labels), where images has shape (batch_size, learning_size, image_size[0], image_size[1], num_channels), and where labels has shape (batch_size, learning_size - 1)

The key difference can be found with "learning_size" in the tensor shape of "images", where "learning_size" represents the number of images being used in parallel for the learning process as seen in (Figure 1). It effectively denotes the kind of architecture it may be, and

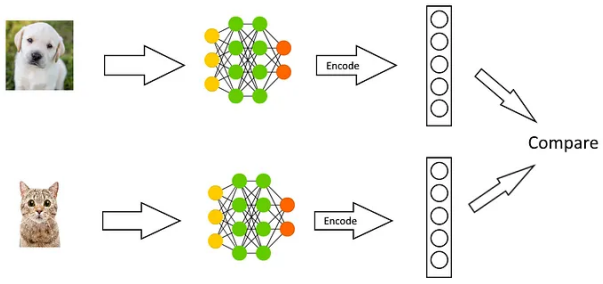


Figure 1: *The basic structure of a Siamese Neural Network, illustrating its parallel nature. Source: [6].*

Figure 2: *An illustration of triplet loss for SiNNs, resulting in a "learning_size" = 3. Source: [6].*

is denoted in other papers as "k" in k-tuplet [7]. For example, it would makes sense for a triplet loss similarity learning architecture, the learning_size would be 3, as there are 3 images being used in parallel for the learning process. However, this variable allows for other architectures to be supported as well.

Additionally, "labels" is changed to a different shape to also allow for other architectures to be supported. For example, if the architecture is a triplet loss similarity learning architecture, the labels would be of shape (batch_size, 2), where the first column represents the similarity of the first image (the anchor) to the second image, and the second column represents the similarity of the first image (the anchor) to the third image. Meanwhile in a case where the learning_size is 2, the labels would be of shape (batch_size, 1), where the first column represents the similarity of the first image (the anchor) to the second image.

Permutation Approach

Function

The initial attempt towards tackling this challenge was anchored in the idea of iterating through the directory, and producing every possible combination of images, this is accomplished by the code in Figure 3.

```
slots = data["files & structure"].keys()
for slot_1 in slots:
    print("Generating data for slot: " + slot_1)
    for file_1 in data["files & structure"][slot_1]:
        for slot_2 in slots:
            for file_2 in data["files & structure"][slot_2]:
                if slot_1 == slot_2:
                    im_1 = np.asarray(Image.open(input_folder_path + slot_1 + "/" + file_1).convert('RGB').resize((64, 64))).tolist()
                    im_2 = np.asarray(Image.open(input_folder_path + slot_2 + "/" + file_2).convert('RGB').resize((64, 64))).tolist()
                    X_train.append([im_1, im_2])
                    Y_train.append(1)
                else:
                    im_1 = np.asarray(Image.open(input_folder_path + slot_1 + "/" + file_1).convert('RGB').resize((64, 64))).tolist()
                    im_2 = np.asarray(Image.open(input_folder_path + slot_2 + "/" + file_2).convert('RGB').resize((64, 64))).tolist()
                    X_train.append([im_1, im_2])
                    Y_train.append(0)
```

Figure 3: *The initial Python code for developing a generator for Siamese Neural Networks.*

Output

The approach illustrated in Figure 3 is a permutation approach, where the generator would iterate through the directory, and produce every possible permutation of images. For example, if the directory had 2 images of class 0, 2 images of class 1, and 2 images of class 2 the generator would produce the following permutations of the images (where p is a positive pair, and n is a negative pair):

Table 4: *Example pairs from the permutation approach*

0:0 + 0:0 p	1:0 + 0:0 n	2:0 + 0:0 n
0:0 + 0:1 p	1:0 + 0:1 n	2:0 + 0:1 n
0:0 + 1:0 n	1:0 + 1:0 p	2:0 + 1:0 n
0:0 + 1:1 n	1:0 + 1:1 p	2:0 + 1:1 n
0:0 + 2:0 n	1:0 + 2:0 n	2:0 + 2:0 p
0:0 + 2:1 n	1:0 + 2:1 n	2:0 + 2:1 p
0:1 + 0:0 p	1:1 + 0:0 n	2:1 + 0:0 n
0:1 + 0:1 p	1:1 + 0:1 n	2:1 + 0:1 n
0:1 + 1:0 n	1:1 + 1:0 p	2:1 + 1:0 n
0:1 + 1:1 n	1:1 + 1:1 p	2:1 + 1:1 n
0:1 + 2:0 n	1:1 + 2:0 n	2:1 + 2:0 p
0:1 + 2:1 n	1:1 + 2:1 n	2:1 + 2:1 p

However, this approach is not scalable. Firstly, this approach does not return a batch of images, but rather the entire dataset. AKA it does not yield sequentially, but rather in one big group. Secondly, this approach will lead to data heavily biased towards dissimilar images due to the nature of permutations. For example, look at a directory database that follows the structure shown in Table 5.

Assuming that within the main directory we see 5 folders representing classes, each with 10 images; With a Tuplet loss, and using 1 singular image of a class as an anchor, we can see that there may only be 10 possible positive cases (including pairing the anchor with itself), and 40 possible negative cases. Of course, as we traverse across the dataset we will acquire additional positive cases, however, the issue of misrepresentation of the dataset is only exacerbated.

Table 5: *Example structure of a tree directory dataset.*

Class		
Index (i)	Identification	Data Count (c[i])
0	Red Oak	10
1	Cedar	10
2	Dogwood	10
3	Maple	10
4	Hickory	10

The formulas for finding such values for one anchor image may be seen below (it should be noted that the (#_of_positives) includes the anchor image being compared to itself):

$$\alpha = (anchor\_class\_index)$$

$$\sigma = (number\_of\_class\_indices)$$

$$c[\alpha] = (anchor\_class\_length) = (\#\_of\_positives)$$

$$(\sum_{i=0}^{\sigma} c[i]) - c[\alpha] = (\#\_of\_negatives)$$

Extending this logic, it is also possible to determine these same values when traversing across the entire dataset (AKA the total positive and negative cases or pairs):

$$\sum_{i=0}^{\sigma}((c[i])^2) = (\#\_of\_positives)$$

$$\sum_{i_1=0}^{\sigma_1}(((\sum_{i_2=0}^{\sigma_2} c[i_2]) - c[\alpha]) * c[\alpha]) = (\#\_of\_negatives)$$

The purpose of appending these formulas to this paper was not only for the sake of explaining the bias towards dissimilar pars or for mathematically explaining each data generator discussed in this paper, but rather to show the scalability of a dataset with similarity learning. Starting with a dataset of only 50 images, a data generator as simple as a permutation approach can produce 2,500 total pairs. The scalability of datasets drastically increases with an increase in the variable that is learning_size. With It is also worth noting that this is entirely in the absence of any data augmentation techniques

Using the general solutions provided by the pervi-ously stated formulas, we can then solve for the specific values of a single anchor image:

$$c[\alpha] = 10$$

$$(\sum_{i=0}^{\sigma} c[i]) - c[\alpha] = 40$$

As well as the values for the entire data set:

$$\sum_{i=0}^{\sigma}((c[i])^2) = 500$$

$$\sum_{i_1=0}^{\sigma_1}(((\sum_{i_2=0}^{\sigma_2} c[i_2]) - c[i_1]) * c[i_1]) = 2000$$

Analysis

Approaching even more complex architectures, more complex data will be required. One example of a more complex system involves a quintuplet learning architecture (Figure 4), another paper covers the usage of such architecture [8]. In order to derive a general solution, the learning_size must be a variable:

Additionally, in the case of smaller datasets, it will lead to a lot of unnecessary loops, especially, if we are interested in getting a unique pair of images, and not one the model has already seen.

The Importance Of Unique Pairs There is, naturally, a belief that it would be good practice to compare an anchor image to itself during similarity training. Obviously, if we did compare an anchor to itself it would

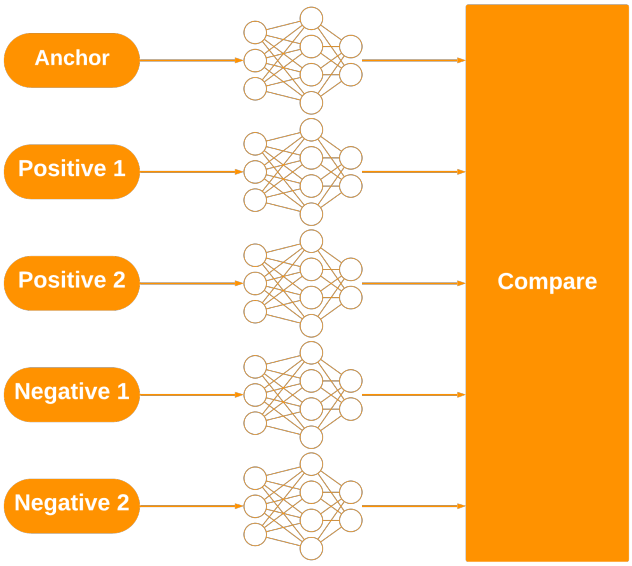


Figure 4: *An illustration of quintuplet architecture, resulting in a "learning_size" = 5.*

be a perfect positive case, with a distance between outputs of the model being 0. However, this leads to an artificial inflation of the accuracy of the model. Figure 5 illustrates the margin that is used in triplet loss very well; If we compare an image to itself, there is no distance between the data points (thus no margin), as they would lie right on top of each other. Therefore, in any model architecture, it is bad practice to compare an image to itself (without any augmentations, as with augmentation, it is not a bad practice).

This can be extended in more complex architectures as well: In a quadruplet loss, you cant have 2 images that are the same, because it will end in a change of embedding that will lean in a way that is unrepresentative of the actual data

The Importance Of Order However, outside of the issue of comparing images to themselves, there is another issue of uniqueness of pairs. In a model architecture where learning_size = 2, there is a potential to have image_1 (as the first image) where it is in a positive pair with image_2 (as the second image). Later on, this pair may be flipped, where image_2 is now the first image, in a positive pair with image_1 as the second image.

The problem of uniqueness or order is reliant then on the loss function and whether or not it is dependant on order. For example, in the case of contrastive loss, both data points are being drawn towards each other (in a positive case), or away from each other (in a negative case) Resulting in the order not mattering. In the case of triplet loss, however, there is not a "side effect of

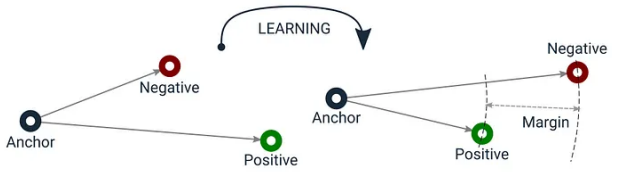


Figure 5: *An illustration of margin as it effects triplet loss. Source: [9].*

urging to encode anchor and positive samples into the same point in the vector space as in Contrastive Loss"[9]. The order of the data being passed to the model does matter, as the anchor is still, where the positive data point is moving towards and the anchor, and the negative is moving away from the anchor.

The reason uniqueness of a pair is important is because if we are interested in training a Siamese Neural Network, we want to ensure that the model is not trained on the same pair of images, as this would lead to the model overfitting to the dataset, and would not be able to generalize well to new data.

So how can we ensure uniqueness? Through a combination approach, this is possible.

Finally, this method doesn't match our requirements, nor does it yield data sequentially, it produces 2 datasets, one being x_train, and the other being y_train.

Combination Approach

Using combinations as opposed to permutations allows for uniqueness, because order doesn't matter in the case of siamese neural networks

$$??? = (\#\_of\_unique\_positives)$$

$$??? = (\#\_of\_unique\_negatives)$$

One-Hot Encoding Approach

Effectively One-Hot Encode data and then compare... this voids the need for for loops, and is entirely based on randomization...

Input positive and negative distribution / proportion (similar to distributing validation and training data)

As well as batch and epoch data

Then randomly select 1 class, and randomly select a value from that class. Then determine if positive or negative pair, and randomly select a corresponding value from that class.

random values may be dependant on whether or not the model has preprocessing layers... (because if they do then you should be able to self compare... AKA comparing an image to itself is only allowed if there is augmentation)

Tensorflow Integration

The "correct" method for integrating software into an open-source project is always up for interpretation. Often times there are several perfectly acceptable methods of producing software, and deciding whether one arbitrary integration over another is a matter of opinion.

In my opinion then, I believe that the best method for integrating this data generator into Tensorflow would be to first compress the many existing data generators that already exist into a single class with several subclasses.

The Mixed Approach (Recommended)

In the mixin approach benefits from its use of subclasses, but eliminates the need for calling the function from the context of a specific generator, by using a single function call. The primary function of the this approach would be:

$$tf.keras.utils.dataset\_from\_directory()$$

Which then takes in a parameter of the generator to be used which would be a subclass of the class **Generators**.

The Subclass Approach

The subclasses are kinds of generators, where (image, text, and audio) are the kinds of data that can be passed to the generator, where one of those is passed as a parameter to the class. In usage, these generators would be called in the **model.fit()** function, as the existing generators are already called.

$$\_.generate(\_.contrastive, learning\_size = 2, ...)$$

This may also be called with:

$$\_.contrastive.generate(learning\_size = 2, ...)$$

```python
print("\n" * 3)
print("Data Generator...")
def train_loop(input_folder_path, Epoch_Size, Batch_Size, X_train_batch = [], Y_train_batch = []):
    # Starting Data
    structure = {}
    for slot in os.listdir(input_folder_path):
        try:
            structure.update({slot: os.listdir(input_folder_path + slot)})
        except:
            pass

    Left_Structure = copy.deepcopy(structure)

    # Batch Control
    epoch_counter = 0
    batch_counter = 0

    while len(Left_Structure.keys()) > 0:

        # Start Loop
        Left_Class, Left_File  = random.choice([(name, value) for name, values in Left_Structure.items() for value in values])
        Right_Structure = copy.deepcopy(structure)


        while len(Right_Structure.keys()) > 0:

            # Start Loop
            Right_Class, Right_File  = random.choice([(name, value) for name, values in Right_Structure.items() for value in values])

            if batch_counter == Batch_Size:
                # Update Epoch Counter
                epoch_counter += 1
                print(str(epoch_counter) + " / " + str(Epoch_Size))

                # Convert to numpy array
                X_train_np_batch = np.array(X_train_batch)
                Y_train_np_batch = np.array(Y_train_batch)

                # print(X_train_np_batch[:, 0].shape)
                print(Y_train_np_batch[:])

                # Train as Epoch
                # Using Multiple model.fit()
                model.fit([X_train_np_batch[:, 0], X_train_np_batch[:, 1]], Y_train_np_batch[:], epochs=1, batch_size=Batch_Size, validation_split=0.1)
                # model.train_on_batch(X, y)
                # model.test_on_batch(X, y)
                # model.fit_generator(data_generator, samples_per_epoch, nb_epoch)
                # print(X_train_np_batch.shape)
                # print(Y_train_np_batch.shape)

                if epoch_counter == Epoch_Size:
                    return "Done, was able to generate the requested data"

                # Reset Batch
                batch_counter = 0
                X_train_batch = []
                Y_train_batch = []

            #TODO: Write a better Div_This function... that allows a range of bias for a dataset...

            def div_this(x, y):
                try:
                    return x / y
                except ZeroDivisionError:
                    return 0

            if (Left_Class == Right_Class) and (div_this(sum(Y_train_batch), len(Y_train_batch)) <= 0.5):
                # Same Class
                im_1 = np.asarray(Image.open(input_folder_path + Left_Class + "/" + Left_File).convert('RGB').resize((64, 64))).tolist()
                im_2 = np.asarray(Image.open(input_folder_path + Right_Class + "/" + Right_File).convert('RGB').resize((64, 64))).tolist()
                X_train_batch.append([im_1, im_2])
                Y_train_batch.append(1)
                batch_counter += 1

                Right_Structure[Right_Class].remove(Right_File)
                if len(Right_Structure[Right_Class]) == 0:
                    Right_Structure.pop(Right_Class)

            elif (Left_Class != Right_Class) and (div_this(sum(Y_train_batch), len(Y_train_batch)) >= 0.5):
                # Different Class
                im_1 = np.asarray(Image.open(input_folder_path + Left_Class + "/" + Left_File).convert('RGB').resize((64, 64))).tolist()
                im_2 = np.asarray(Image.open(input_folder_path + Right_Class + "/" + Right_File).convert('RGB').resize((64, 64))).tolist()
                X_train_batch.append([im_1, im_2])
                Y_train_batch.append(0)
                batch_counter += 1

                Right_Structure[Right_Class].remove(Right_File)
                if len(Right_Structure[Right_Class]) == 0:
                    Right_Structure.pop(Right_Class)

            else:
                Right_Structure[Right_Class].remove(Right_File)
                if len(Right_Structure[Right_Class]) == 0:
                    Right_Structure.pop(Right_Class)


        # Finish Loop
        Left_Structure[Left_Class].remove(Left_File)
        if len(Left_Structure[Left_Class]) == 0:
            Left_Structure.pop(Left_Class)


    train_loop(input_folder_path, Epoch_Size - epoch_counter, Batch_Size, )

    # Training sequence
    print(train_loop(input_folder_path, 50, 100))
```

Figure 6: *The second Python script for developing a generator for Siamese Neural Networks.*

The Mixin Approach

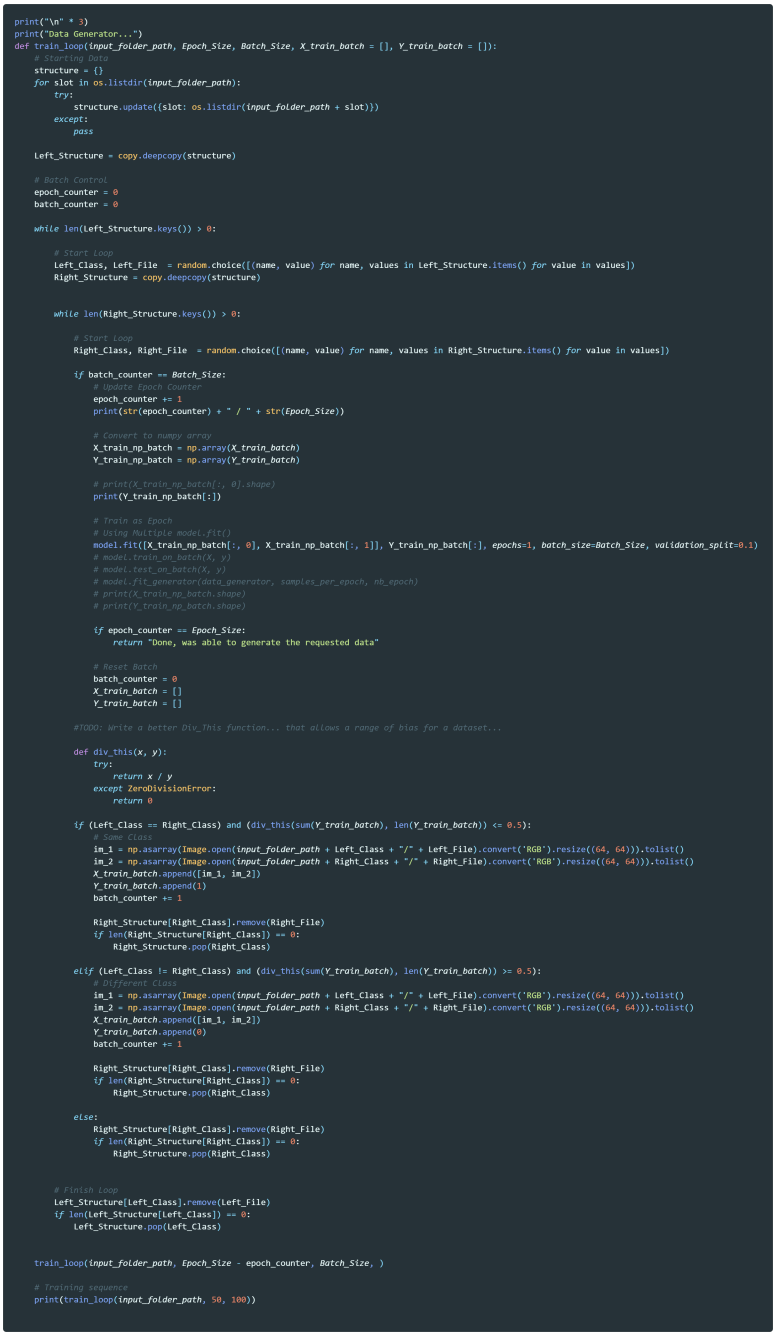
The Dictionary Approach

The args Approach

The String Approach

References

[1] Gil Press. "A Very Short History Of Artificial Intelligence". In: *Forbes* (Oct. 2022). URL: https://



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                # print(X_train_np_batch[:, 0].shape)
                print(Y_train_np_batch[:])

                # Train as Epoch
                # Using Multiple model.fit()
                model.fit([X_train_np_batch[:, 0], X_train_np_batch[:, 1]], Y_train_np_batch[:], epochs=1, batch_size=Batch_Size, validation_split=0.1)
                # model.train_on_batch(X, y)
                # model.test_on_batch(X, y)
                # model.fit_generator(data_generator, samples_per_epoch, nb_epoch)
                # print(X_train_np_batch.shape)
                # print(Y_train_np_batch.shape)

                if epoch_counter == Epoch_Size:
                    return "Done, was able to generate the requested data"

                # Reset Batch
                batch_counter = 0
                X_train_batch = []
                Y_train_batch = []

            #TODO: Write a better Div_This function... that allows a range of bias for a dataset...

            def div_this(x, y):
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                # Same Class
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                im_2 = np.asarray(Image.open(input_folder_path + Right_Class + "/" + Right_File).convert('RGB').resize((64, 64))).tolist()
                X_train_batch.append([im_1, im_2])
                Y_train_batch.append(1)
                batch_counter += 1

                Right_Structure[Right_Class].remove(Right_File)
                if len(Right_Structure[Right_Class]) == 0:
                    Right_Structure.pop(Right_Class)

            elif (Left_Class != Right_Class) and (div_this(sum(Y_train_batch), len(Y_train_batch)) >= 0.5):
                # Different Class
                im_1 = np.asarray(Image.open(input_folder_path + Left_Class + "/" + Left_File).convert('RGB').resize((64, 64))).tolist()
                im_2 = np.asarray(Image.open(input_folder_path + Right_Class + "/" + Right_File).convert('RGB').resize((64, 64))).tolist()
                X_train_batch.append([im_1, im_2])
                Y_train_batch.append(0)
                batch_counter += 1

                Right_Structure[Right_Class].remove(Right_File)
                if len(Right_Structure[Right_Class]) == 0:
                    Right_Structure.pop(Right_Class)

            else:
                Right_Structure[Right_Class].remove(Right_File)
                if len(Right_Structure[Right_Class]) == 0:
                    Right_Structure.pop(Right_Class)


        # Finish Loop
        Left_Structure[Left_Class].remove(Left_File)
        if len(Left_Structure[Left_Class]) == 0:
            Left_Structure.pop(Left_Class)


    train_loop(input_folder_path, Epoch_Size - epoch_counter, Batch_Size, )

    # Training sequence
    print(train_loop(input_folder_path, 50, 100))
```

Figure 7: *The second Python script for developing a generator for Siamese Neural Networks.*

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