PyTorch Metric Learning

Kevin Musgrave  
*Cornell Tech*

Serge Belongie  
*Cornell Tech*

Ser-Nam Lim  
*Facebook AI*

Abstract

Deep metric learning algorithms have a wide variety of applications, but implementing these algorithms can be tedious and time consuming. PyTorch Metric Learning is an open source library that aims to remove this barrier for both researchers and practitioners. The modular and flexible design allows users to easily try out different combinations of algorithms in their existing code. It also comes with complete train/test workflows, for users who want results fast. Code and documentation is available at github.com/KevinMusgrave/pytorch-metric-learning.

1. Design

Figure 1 gives a high-level view of how the main modules relate to each other. Note that each module can be used independently within an existing codebase, or combined together for a complete train/test workflow. The following sections cover each module in detail.

Figure 1: High level view of the library’s main modules, with simplified pseudo code.
1.1 Losses

Loss functions work similarly to many regular PyTorch loss functions, in that they operate on a two-dimensional tensor and its corresponding labels:

```python
from pytorch_metric_learning.losses import NTXentLoss
loss_func = NTXentLoss()
### training loop ###
for data, labels in dataloader:
    embeddings = model(data)
    loss = loss_func(embeddings, labels)
    loss.backward()
```

But as shown in Figure 2, loss functions can be augmented through the use of miners, distances, regularizers, and reducers. First consider distances: all losses operate on a distance matrix, whether it is the distances between each pair of embeddings in a batch, or between embeddings and learned weights. So internally, the loss function uses a distance object to compute a pairwise distance matrix, and then uses elements of this matrix to compute the loss.

![Distance Matrix and Indices](image)

**Figure 2:** The components of a loss function. In this illustration, a miner finds the indices of hard pairs in the current batch. These are used to index into the distance matrix, computed by the distance object. For this example, the loss function is pair-based, so it computes a loss per pair. In addition, a regularizer has been supplied, so a regularization loss is computed for each embedding in the batch. The per-pair and per-element losses are passed to the reducer, which (in this example) only keeps losses with a high value. The averages are computed for the high-valued pair and element losses, and are then added together to obtain the final loss.
1.2 Distances

As an example of how distance objects work, consider the TripletMarginLoss with its default distance metric:

```python
from pytorch_metric_learning.losses import TripletMarginLoss
loss_func = TripletMarginLoss()
```

In this form, the loss computes the following for every triplet in the batch:

\[ L_{\text{triplet}} = [d_{ap} - d_{an} + \text{margin}]_+ \]

where \( d \) is Euclidean distance. This distance metric can be replaced by passing in a different distance object:

```python
from pytorch_metric_learning.losses import TripletMarginLoss
from pytorch_metric_learning.distances import SNRDistance
loss_func = TripletMarginLoss(distance = SNRDistance())
```

Now \( d \) represents the signal to noise ratio. The same loss function can also be used with inverted distance metrics, such as cosine similarity:

```python
from pytorch_metric_learning.losses import TripletMarginLoss
from pytorch_metric_learning.distances import CosineSimilarity
loss_func = TripletMarginLoss(distance = CosineSimilarity())
```

Even though CosineSimilarity is an inverted metric (large values indicate higher similarity), the loss function still works because it internally makes the necessary adjustments for the calculation to make sense. Specifically, the TripletMarginLoss swaps the anchor-positive and anchor-negative terms:

\[ L_{\text{triplet}} = [s_{an} - s_{ap} + \text{margin}]_+ \]

where \( s \) is cosine similarity.

All losses, miners, and regularizers accept a distance argument. This makes it very easy to try out different combinations, like the MultiSimilarityMiner using SNRDistance, or the NTXentLoss using LpDistance(p=1) and so on. Note that some losses/miners/regularizers have restrictions on the type of distances they can accept. For example, some classification losses only allow CosineSimilarity or DotProductSimilarity as their distance measure between embeddings and weights. These details are available in the documentation.

1.3 Reducers

Losses are typically computed per element, pair, or triplet, and are then reduced to a single value by some operation, such as averaging. Many PyTorch loss functions accept a reduction parameter, which is usually either "mean", "sum", or "none". In PyTorch Metric Learning, the reducer parameter serves a similar purpose, but with increased modularity and functionality. Specifically, a reducer object operates on a dictionary which describes the losses, and then returns the reduced value. For maximum flexibility, a reducer can be
written to operate differently for per-element, per-pair, and per-triplet losses. Here is an example of how to pass a reducer to a loss function:

```python
from pytorch_metric_learning.losses import MultiSimilarityLoss
from pytorch_metric_learning.reducers import ThresholdReducer
loss_func = MultiSimilarityLoss(reducer = ThresholdReducer(low = 10, high = 30))
```

The ThresholdReducer will discard all losses that fall below low and above high, and then return the average of the remaining losses.

### 1.4 Regularizers

It is common to add embedding or weight regularization terms to the core metric learning loss. This is straightforward to do, because every loss function has an optional embedding_regularizer parameter:

```python
from pytorch_metric_learning.losses import ContrastiveLoss
from pytorch_metric_learning.regularizers import LpRegularizer
loss_func = ContrastiveLoss(embedding_regularizer = LpRegularizer())
```

In addition, classification losses have an optional weight_regularizer parameter:

```python
from pytorch_metric_learning.losses import ArcFaceLoss
from pytorch_metric_learning.regularizers import RegularFaceRegularizer
loss_func = ArcFaceLoss(weight_regularizer = RegularFaceRegularizer())
```

The corresponding loss multipliers are specified by embedding_reg_weight and weight_reg_weight.

### 1.5 Miners

An important concept in metric learning is mining, which is the process of finding the best samples to train on. Miners come in two flavors: online miners, which find the best tuples within an already sampled batch, and offline miners, which determine the best way to create batches. In this library, online miners are part of the miners module, while offline miners are planned to be implemented in the samplers module. It is easy to use an online miner in conjunction with a loss function:

```python
from pytorch_metric_learning.losses import CircleLoss
from pytorch_metric_learning.miners import MultiSimilarityMiner
loss_func = CircleLoss()
mining_func = MultiSimilarityMiner()
## training loop ##
for data, labels in dataloader:
    embeddings = model(data)
    hard_tuples = mining_func(embeddings, labels)
    loss = loss_func(embeddings, labels, hard_tuples)
    loss.backward()
```
In the above snippet, MultiSimilarityMiner finds the hard pairs within each batch, and passes the indices of those hard pairs to the loss function. The loss will then be computed using only those pairs. But what happens if the loss function operates on triplets and not pairs? This will still work, because the library converts tuples if necessary. Specifically:

- If pairs are passed into a triplet loss, then triplets will be formed by combining each positive pair and negative pair that share the same anchor.
- If triplets are passed into a pair loss, then pairs will be formed by splitting each triplet into two pairs.
- If pairs or triplets are passed into a classification loss, then each embedding’s loss will be weighted by how frequently the embedding occurs in the pairs or triplets.

1.6 Samplers

Samplers in this library are the same as PyTorch samplers, in that they are passed to data loaders, and determine how batches are formed. Currently this module serves more as a utility than as a bank of algorithms, but in the future it will contain offline miners.

1.7 Trainers

Trainers exist in this library because some metric learning algorithms are more than just losses or mining functions. Some algorithms require additional networks, data augmentations, learning rate schedules etc. The goal of the trainers module is to provide access to these types of metric learning algorithms. In general, trainers make minimal assumptions, only taking care of the forward/backward pass, while leaving the choice of model, loss functions, optimizers etc. to the user. In addition, trainers have end-of-iteration and end-of-epoch hooks for further customizability.

1.8 Testers

Given a model and a dataset, a tester computes the embeddings, applies any specified transformations, creates visualizations of the embedding space, and determines the accuracy of the model. Accuracy calculations are performed by the aptly named AccuracyCalculator class. Thus, users can easily create their own accuracy metrics by passing in a custom AccuracyCalculator object.

1.9 Accuracy Calculation

The default AccuracyCalculator computes accuracy via its get_accuracy function, and is based on k-means clustering and k-nearest neighbors (k-nn). The clustering results are used to compute Adjusted Mutual Information (AMI) and Normalized Mutual Information (NMI), while the k-nn results are used to compute Precision@1, R-Precision, and MAP@R. The output is a dictionary mapping from metric names to values.

Writing a custom accuracy calculator is straightforward, due to the amount of boilerplate that is already provided in the parent class. Here is an example of adding a new Custom Mutual Information metric:
from pytorch_metric_learning.utils import import accuracy_calculator

class CustomCalculator(accuracy_calculator.AccuracyCalculator):
    def calculate_CMI(self, query_labels, cluster_labels, **kwargs):
        return some_complicated_function(query_labels, cluster_labels)

    def requires_clustering(self):
        return super().requires_clustering() + ['CMI']

Now CMI will be included in the output dictionary. This custom calculator can be used independently, or it can be passed into a tester object:

from pytorch_metric_learning import import testers
t = testers.GlobalEmbeddingSpaceTester(accuracy_calculator=CustomCalculator())

1.10 Hooks
As mentioned previously, trainers contain hooks that allow users to customize the end-of-iteration and end-of-epoch behavior. For users who are short of time, this library comes with the HookContainer class, which essentially converts trainers into a complete train/test workflow, with logging and model saving.

2. Related libraries
Other open source metric learning libraries include metric-learn (de Vazelhes et al. (2020)) and pyDML (Suarez et al. (2020)). However, their focus is on classic metric learning algorithms, using numpy (Walt et al. (2011)) and scikit-learn (Pedregosa et al. (2011)). In contrast, our library focuses on deep metric learning, and uses PyTorch (Paszke et al. (2019)) as its backbone.

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