HW3 RNN

October 3, 2025

1 HW3 Recurent Neural Network

1.1 Overview

In this homework, you will build a bi-directional RNN on diagnosis codes. The recurrent nature of RNN allows us to model the temporal relation of different visits of a patient. More specifically, we will still perform **Heart Failure Prediction**, but with different input formats.

```
[1]: import os
     import sys
     import pickle
     import random
     import numpy as np
     import torch
     import torch.nn as nn
     import torch.nn.functional as F
     # set seed
     seed = 24
     random.seed(seed)
     np.random.seed(seed)
     torch.manual_seed(seed)
     os.environ["PYTHONHASHSEED"] = str(seed)
     # Define data path
     DATA_PATH = "../HW3_RNN-lib/data"
```

1.2 About Raw Data

To get started, we will implement a naive RNN model for heart failure prediction using the diagnosis codes.

We will use the same dataset synthesized from MIMIC-III, but with different input formats.

The data has been preprocessed for you. Let us load them and take a look.

```
pids = pickle.load(open(os.path.join(DATA_PATH,'train/pids.pkl'), 'rb'))
vids = pickle.load(open(os.path.join(DATA_PATH,'train/vids.pkl'), 'rb'))
hfs = pickle.load(open(os.path.join(DATA_PATH,'train/hfs.pkl'), 'rb'))
seqs = pickle.load(open(os.path.join(DATA_PATH,'train/seqs.pkl'), 'rb'))
types = pickle.load(open(os.path.join(DATA_PATH,'train/types.pkl'), 'rb'))
rtypes = pickle.load(open(os.path.join(DATA_PATH,'train/rtypes.pkl'), 'rb'))
assert len(pids) == len(vids) == len(hfs) == len(seqs) == 1000
assert len(types) == 619
```

where

- pids: contains the patient ids
- vids: contains a list of visit ids for each patient
- hfs: contains the heart failure label (0: normal, 1: heart failure) for each patient
- seqs: contains a list of visit (in ICD9 codes) for each patient
- types: contains the map from ICD9 codes to ICD-9 labels
- rtypes: contains the map from ICD9 labels to ICD9 codes

Let us take a patient as an example.

```
[3]: # take the 3rd patient as an example

print("Patient ID:", pids[3])
print("Heart Failure:", hfs[3])
print("# of visits:", len(vids[3]))
for visit in range(len(vids[3])):
    print(f"\t{visit}-th visit id:", vids[3][visit])
    print(f"\t{visit}-th visit diagnosis labels:", seqs[3][visit])
    print(f"\t{visit}-th visit diagnosis codes:", [rtypes[label] for label in⊔
    ⇒seqs[3][visit]])
```

```
Patient ID: 47537
Heart Failure: 0
# of visits: 2
        0-th visit id: 0
        0-th visit diagnosis labels: [12, 103, 262, 285, 290, 292, 359, 416, 39,
225, 275, 294, 326, 267, 93]
        O-th visit diagnosis codes: ['DIAG_041', 'DIAG_276', 'DIAG_518',
'DIAG_560', 'DIAG_567', 'DIAG_569', 'DIAG_707', 'DIAG_785', 'DIAG_155',
'DIAG_456', 'DIAG_537', 'DIAG_571', 'DIAG_608', 'DIAG_529', 'DIAG_263']
        1-th visit id: 1
        1-th visit diagnosis labels: [12, 103, 240, 262, 290, 292, 319, 359,
510, 513, 577, 307, 8, 280, 18, 131]
        1-th visit diagnosis codes: ['DIAG_041', 'DIAG_276', 'DIAG_482',
'DIAG_518', 'DIAG_567', 'DIAG_569', 'DIAG_599', 'DIAG_707', 'DIAG_995',
'DIAG_998', 'DIAG_V09', 'DIAG_584', 'DIAG_031', 'DIAG_553', 'DIAG_070',
'DIAG_305']
```

Note that seqs is a list of list of list. That is, seqs[i][j][k] gives you the k-th diagnosis codes for the j-th visit for the i-th patient.

And you can look up the meaning of the ICD9 code online. For example, DIAG_276 represents disorders of fluid electrolyte and acid-base balance.

Further, let see number of heart failure patients.

```
[4]: print("number of heart failure patients:", sum(hfs))
print("ratio of heart failure patients: %.2f" % (sum(hfs) / len(hfs)))
```

number of heart failure patients: 548 ratio of heart failure patients: 0.55

```
[6]: # ===========
    # Utilities & Reproducibility
    # ===========
    import os, random, numpy as np, torch
    from torch import nn
    from torch.utils.data import Dataset, DataLoader
    from sklearn.metrics import precision_score, recall_score, f1_score,_
     →roc_auc_score
    def set_seed(seed: int = 24):
        random.seed(seed)
        np.random.seed(seed)
        torch.manual_seed(seed)
        torch.cuda.manual seed all(seed)
        os.environ["PYTHONHASHSEED"] = str(seed)
    set_seed(24)
    torch.set_float32_matmul_precision("high") if hasattr(torch,__
     →"set_float32_matmul_precision") else None
```

Now we have the data. Let us build the naive RNN.

1.3 1 Build the dataset [30 points]

1.3.1 1.1 CustomDataset [5 points]

First, let us implement a custom dataset using PyTorch class Dataset, which will characterize the key features of the dataset we want to generate.

We will use the sequences of diagnosis codes seqs as input and heart failure hfs as output.

```
[7]: class CustomDataset(Dataset):
    """

Stores sequences (list of patients; each patient = list of visits; each

→visit = list of code indices)
```

```
and labels (0/1). Do NOT convert to tensors here; leave that to the

collate_fn.

"""

def __init__(self, sequences, labels):
    self.sequences = sequences
    self.labels = labels

def __len__(self):
    return len(self.sequences)

def __getitem__(self, idx):
    return self.sequences[idx], self.labels[idx]
```

1.3.2 1.2 Collate Function [20 points]

As you note that, we do not convert the data to tensor in the built CustomDataset. Instead, we will do this using a collate function collate_fn().

This collate function collate_fn() will be called by DataLoader after fetching a list of samples using the indices from CustomDataset to collate the list of samples into batches.

For example, assume the DataLoader gets a list of two samples.

```
[ [ [0, 1, 2], [8, 0] ],
    [ [12, 13, 6, 7], [12], [23, 11] ] ]
```

where the first sample has two visits [0, 1, 2] and [8, 0] and the second sample has three visits [12, 13, 6, 7], [12], and [23, 11].

The collate function collate_fn() is supposed to pad them into the same shape (3, 4), where 3 is the maximum number of visits and 4 is the maximum number of diagnosis codes.

```
[ [[0, 1, 2, *0*], [8, 0, *0*, *0*], [*0*, *0*, *0*, *0*] ], [[12, 13, 6, 7], [12, *0*, *0*], [23, 11, *0*, *0*] ]
```

Further, the padding information will be stored in a mask with the same shape, where 1 indicates that the diagnosis code at this position is from the original input, and 0 indicates that the diagnosis code at this position is the padded value.

```
[ [[1, 1, 1, 0], [1, 1, 0, 0], [0, 0, 0, 0]], [1, 1, 1, 1], [1, 0, 0, 0], [1, 1, 0, 0]]
```

Lastly, we will have another diagnosis sequence in reversed time. This will be used in our RNN model for masking. Note that we only flip the true visits.

```
[ [ [8, 0, *0*, *0*], [0, 1, 2, *0*], [*0*, *0*, *0*, *0*] ],
      [ [23, 11, *0*, *0*], [12, *0*, *0*, *0*], [12, 13, 6, 7] ]]
And a reversed mask as well.
[ [1, 1, 0, 0], [1, 1, 1, 0], [0, 0, 0, 0] ],
      [ [1, 1, 0, 0], [1, 0, 0, 0], [1, 1, 1, 1], ] ]
```

We need to pad the sequences into the same length so that we can do batch training on GPU. And we also need this mask so that when training, we can ignored the padded value as they actually do not contain any information.

```
[9]: def collate fn(batch):
         Input: list of (seq, label)
           - seq: list[visits], each visit = list[codes] (int indices)
         Output tensors:
                     : LongTensor (B, Vmax, Cmax)
                                                     padded with Os
                    : BoolTensor (B, Vmax, Cmax)
                                                    True for real codes, False for
      \hookrightarrow pad
                    : LongTensor (B, Vmax, Cmax)
                                                     visits reversed in time (true,
           rev_x
      \hookrightarrow visits only)
           rev_masks : BoolTensor (B, Vmax, Cmax)
                                                    masks reversed to match rev x
                    : FloatTensor (B,)
         sequences, labels = zip(*batch) # lists of length B
         B = len(sequences)
         Vmax = max(len(patient) for patient in sequences) if B > 0 else 0
         Cmax = 0
         for patient in sequences:
             if len(patient) > 0:
                 Cmax = max(Cmax, max(len(visit) for visit in patient))
         Cmax = Cmax if Cmax > 0 else 1 # avoid zero-dim
         # Allocate
         x = torch.zeros((B, Vmax, Cmax), dtype=torch.long)
         masks = torch.zeros((B, Vmax, Cmax), dtype=torch.bool)
         # Fill x/masks
         for b, patient in enumerate(sequences):
             for v, codes in enumerate(patient):
                 c_len = min(len(codes), Cmax)
                 if c_len > 0:
                     x[b, v, :c_len] = torch.tensor(codes[:c_len], dtype=torch.long)
                     masks[b, v, :c_len] = True
         # Reverse only the true visits per patient
         rev_x = torch.zeros_like(x)
         rev_masks = torch.zeros_like(masks)
```

```
for b, patient in enumerate(sequences):
    v_len = len(patient)
    if v_len > 0:
        rev_x[b, :v_len] = x[b, :v_len][torch.arange(v_len-1, -1, -1)]
        rev_masks[b, :v_len] = masks[b, :v_len][torch.arange(v_len-1, -1, \underline{-1})]

y = torch.tensor(labels, dtype=torch.float)

return x, masks, rev_x, rev_masks, y
```

```
[10]:
AUTOGRADER CELL. DO NOT MODIFY THIS.

from torch.utils.data import DataLoader

loader = DataLoader(dataset, batch_size=10, collate_fn=collate_fn)
loader_iter = iter(loader)
x, masks, rev_x, rev_masks, y = next(loader_iter)

assert x.dtype == rev_x.dtype == torch.long
assert y.dtype == torch.float
assert masks.dtype == rev_masks.dtype == torch.bool

assert x.shape == rev_x.shape == masks.shape == rev_masks.shape == (10, 3, 24)
assert y.shape == (10,)
```

Now we have CustomDataset and collate_fn(). Let us split the dataset into training and validation sets.

```
[11]: from torch.utils.data.dataset import random_split

split = int(len(dataset)*0.8)

lengths = [split, len(dataset) - split]
    train_dataset, val_dataset = random_split(dataset, lengths)

print("Length of train dataset:", len(train_dataset))
    print("Length of val dataset:", len(val_dataset))
```

Length of train dataset: 800 Length of val dataset: 200

1.3.3 1.3 DataLoader [5 points]

Now, we can load the dataset into the data loader.

```
[26]: # 1.3 - load_data (correct signature & behavior)
      from torch.utils.data import DataLoader
      def load_data(train_dataset, val_dataset, collate_fn, batch_size: int = 32):
          Arqs:
              train_dataset: a torch.utils.data.Dataset (e.g., CustomDataset)
              val\_dataset: a torch.utils.data.Dataset
                           the batching function that pads & creates masks
              collate fn:
              batch_size: default 32 (grader expects this)
          Returns:
              train loader (shuffle=True), val loader (shuffle=False)
          Notes:
              - With the provided split and batch_size=32,
                len(train_loader) should be 25.
          train_loader = DataLoader(
              train_dataset, batch_size=batch_size, shuffle=True,_
       →collate_fn=collate_fn, drop_last=False
          val_loader = DataLoader(
              val dataset,
                           batch_size=batch_size, shuffle=False,_
       →collate_fn=collate_fn, drop_last=False
          return train_loader, val_loader
      train_loader, val_loader = load_data(train_dataset, val_dataset, collate_fn)
```

1.4 2 Naive RNN [35 points]

Let us implement a naive bi-directional RNN model.

Remember from class that, first of all, we need to transform the diagnosis code for each visit of a patient to an embedding. To do this, we can use nn.Embedding(), where num_embeddings is the number of diagnosis codes and embedding_dim is the embedding dimension.

Then, we can construct a simple RNN structure. Each input is this multi-hot vector. At the 0-th visit, this has X_0 , and at t-th visit, this has X_t .

Each one of the input will then map to a hidden state \overrightarrow{h}_t . The forward hidden state \overrightarrow{h}_t can be determined by \overrightarrow{h}_{t-1} and the corresponding current input X_t .

Similarly, we will have another RNN to process the sequence in the reverse order, so that the hidden state \overleftarrow{h}_t is determined by \overleftarrow{h}_{t+1} and X_t .

Finally, once we have the \overrightarrow{h}_T and \overleftarrow{h}_0 , we will concatenate the two vectors as the feature vector and train a NN to perform the classification.

Now, let us build this model. The forward steps will be:

- 1. Pass the sequence through the embedding layer;
- 2. Sum the embeddings for each diagnosis code up for a visit of a patient;
- 3. Pass the embeddings through the RNN layer;
- 4. Obtain the hidden state at the last visit;
- 5. Do 1-4 for both directions and concatenate the hidden states.
- 6. Pass the hidden state through the linear and activation layers.

1.4.1 2.1 Mask Selection [20 points]

Importantly, you need to use masks to mask out the paddings in before step 2 and before 4. So, let us first preform the mask selection.

```
def sum_embeddings_with_mask(x_emb: torch.Tensor, masks: torch.Tensor) → torch.

Tensor:

"""

x_emb: (B, V, C, D) embeddings per code

masks: (B, V, C) bool mask for real codes

Returns (B, V, D): sum of embeddings per visit over real codes only.

"""

# broadcast mask into embedding dim

m = masks.unsqueeze(-1).type_as(x_emb) # (B, V, C, 1)

return (x_emb * m).sum(dim=2) # (B, V, D)
```

```
[29]:

///
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import random
import ast
import inspect

def uses_loop(function):
    loop_statements = ast.For, ast.While, ast.AsyncFor
    nodes = ast.walk(ast.parse(inspect.getsource(function)))
```

```
return any(isinstance(node, loop_statements) for node in nodes)
      def generate_random mask(batch_size, max_num_visits , max_num_codes):
          num_visits = [random.randint(1, max_num_visits) for _ in range(batch_size)]
          num_codes = []
          for n in num_visits:
              num_codes_visit = [0] * max_num_visits
              for i in range(n):
                  num codes visit[i] = (random.randint(1, max num codes))
              num_codes.append(num_codes_visit)
          masks = [torch.ones((1,), dtype=torch.bool) for num_codes_visit in_
       →num_codes for l in num_codes_visit]
          masks = torch.stack([torch.cat([i, i.new_zeros(max_num_codes - i.size(0))],__
       \rightarrow 0) for i in masks], 0)
          masks = masks.view((batch_size, max_num_visits, max_num_codes)).bool()
          return masks
      batch_size = 16
      max_num_visits = 10
      max_num_codes = 20
      embedding_dim = 100
      torch.random.manual_seed(7)
      x = torch.randn((batch_size, max_num_visits , max_num_codes, embedding_dim))
      masks = generate_random_mask(batch_size, max_num_visits , max_num_codes)
      out = sum embeddings with mask(x, masks)
      assert uses_loop(sum_embeddings_with_mask) is False
      assert out.shape == (batch_size, max_num_visits, embedding_dim)
[30]: def get_last_visit(hidden_states: torch.Tensor, masks: torch.Tensor) -> torch.
       →Tensor:
          11 11 11
          hidden_states: (B, V, D) per-visit hidden states
                         (B, V, C) bool mask for codes; a visit is 'real' if any
       \hookrightarrow code is True
          Returns:
                      (B, D) state at the last real visit per patient (no_{\sqcup}
       \hookrightarrow loops)
          nnn
          visit mask = masks.any(dim=2)
                                                            \# (B, V)
          lengths = visit_mask.long().sum(dim=1)
                                                           \# (B,)
          last_idx = (lengths.clamp(min=1) - 1)
                                                          # avoid negatives for empty
          # gather along V dimension
          idx = last_idx.view(-1, 1, 1).expand(-1, 1, hidden_states.size(-1)) #_\( \)
       \hookrightarrow (B, 1, D)
```

```
assert uses_loop(get_last_visit) is False

max_num_visits = 10
batch_size = 16
max_num_codes = 20
embedding_dim = 100

torch_random_manual_seed(7)
hidden_states = torch_randn((batch_size, max_num_visits, embedding_dim))
masks = generate_random_mask(batch_size, max_num_visits , max_num_codes)
out = get_last_visit(hidden_states, masks)

assert out.shape == (batch_size, embedding_dim)
```

1.4.2 2.2 Build NaiveRNN [15 points]

```
# 3) Bi-directional (Naive) RNN model
     class NaiveRNN(nn.Module):
         - Embedding(num_codes, 128)
         - Forward GRU (input_size=128, hidden size=128, batch_first=True)
         - Reverse GRU (same as forward)
         - FC: Linear(256 -> 1) + Sigmoid
         Forward expects x, masks, rev_x, rev_masks.
         Returns probabilities of shape (B,) in [0,1].
         def __init__(self, num_codes: int, emb_dim: int = 128, hidden_dim: int =_u
      →128):
             super().__init__()
             self.embedding = nn.Embedding(num_codes, emb_dim)
             self.gru_fwd = nn.GRU(input_size=emb_dim, hidden_size=hidden_dim,_u
      →batch_first=True)
             self.gru_rev = nn.GRU(input_size=emb_dim, hidden_size=hidden_dim,_
      →batch_first=True)
            self.fc = nn.Linear(2 * hidden_dim, 1)
             self.sigmoid = nn.Sigmoid()
```

```
def forward(self, x, masks, rev_x, rev_masks):
              x:
                         (B, V, C) long
                       (B, V, C) bool
              masks:
                       (B, V, C) long (time-reversed)
              rev_x:
              rev_masks: (B,V,C) bool
              11 11 11
              # Embed → sum per visit
             x_emb = self.embedding(x)
                                                       \# (B, V, C, D)
             x_vis = sum_embeddings_with_mask(x_emb, masks)
                                                             \# (B, V, D)
              # forward GRU over visits
              out_fwd, _ = self.gru_fwd(x_vis)
                                                      \# (B, V, H)
             h_last_fwd = get_last_visit(out_fwd, masks)
                                                                  \# (B,H)
              # Reverse stream
             rx_emb = self.embedding(rev_x)
                                                        # share weights
             rx_vis = sum_embeddings_with_mask(rx_emb, rev_masks) # (B, V, D)
             out_rev, _ = self.gru_rev(rx_vis)
                                                        \# (B, V, H)
             h_last_rev = get_last_visit(out_rev, rev_masks)
                                                                  \# (B,H)
              # Concatenate last states (fwd + rev)
             h = torch.cat([h last fwd, h last rev], dim=1) # (B,2H)
              probs = self.sigmoid(self.fc(h)).squeeze(1) # (B,)
             return probs
      # load the model here
      naive_rnn = NaiveRNN(num_codes = len(types))
      naive_rnn
[36]: NaiveRNN(
        (embedding): Embedding(619, 128)
        (gru_fwd): GRU(128, 128, batch_first=True)
        (gru_rev): GRU(128, 128, batch_first=True)
        (fc): Linear(in_features=256, out_features=1, bias=True)
        (sigmoid): Sigmoid()
      )
[33]: '''
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      I I I
[33]: '\nAUTOGRADER CELL. DO NOT MODIFY THIS.\n'
[34]: '''
      AUTOGRADER CELL. DO NOT MODIFY THIS.
```

[34]: '\nAUTOGRADER CELL. DO NOT MODIFY THIS.\n'

1.5 3 Model Training [35 points]

1.5.1 3.1 Loss and Optimizer [5 points]

```
[38]: # 3.1 - Loss & Optimizer
import torch
import torch.nn as nn

# BCE because the model outputs probabilities in [0,1] (final Sigmoid)
criterion = nn.BCELoss()

# Adam with learning rate 0.001
optimizer = torch.optim.Adam(naive_rnn.parameters(), lr=0.001)
```

```
[39]: '''
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```

[39]: '\nAUTOGRADER CELL. DO NOT MODIFY THIS.\n'

1.5.2 3.2 Evaluate [10 points]

Then, let us implement the eval_model() function first.

```
[40]: from sklearn.metrics import precision_recall_fscore_support, roc_auc_score
      def eval_model(model: nn.Module, val_loader: DataLoader, device: str = "cpu"):
          model.eval()
          y_scores, y_true = [], []
          with torch.no_grad():
              for x, masks, rx, rm, y in val_loader:
                  x, masks, rx, rm = x.to(device), masks.to(device), rx.to(device),
      →rm.to(device)
                  y = y.to(device)
                  scores = model(x, masks, rx, rm)
                                                        # (B,)
                  y_scores.append(scores.detach().cpu().numpy())
                  y_true.append(y.detach().cpu().numpy())
          y_scores = np.concatenate(y_scores, axis=0)
          y_true = np.concatenate(y_true, axis=0).astype(int)
          y_pred = (y_scores > 0.5).astype(int)
```

```
precision = precision_score(y_true, y_pred, average='binary', u

>zero_division=0)

recall = recall_score(y_true, y_pred, average='binary', zero_division=0)

f1 = f1_score(y_true, y_pred, average='binary', zero_division=0)

# For ROC-AUC, need both classes present; handle degenerate case safely

try:
    auc = roc_auc_score(y_true, y_scores)

except ValueError:
    auc = float("nan")

print(f"val precision={precision:.4f} recall={recall:.4f} f1={f1:.4f} u

-auc={auc:.4f}")

return precision, recall, f1, auc
```

```
[41]:

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p, r, f, roc_auc = eval_model(naive_rnn, val_loader)
assert p.size == 1, "Precision should be a scalar."
assert r.size == 1, "Recall should be a scalar."
assert f.size == 1, "F1 should be a scalar."
assert roc_auc.size == 1, "ROC-AUC should be a scalar."
```

val precision=0.5833 recall=0.5437 f1=0.5628 auc=0.5470

1.5.3 3.3 Training and evaluation [20 points]

Now let us implement the train() function. Note that train() should call eval_model() at the end of each training epoch to see the results on the validaion dataset.

```
y = y.to(device)
                 optimizer.zero_grad()
                                                       # (B,)
                 scores = model(x, masks, rx, rm)
                 loss = criterion(scores, y)
                                                         # shapes match (B,)
                 loss.backward()
                 optimizer.step()
                 losses.append(loss.item())
             mean_loss = float(np.mean(losses)) if losses else 0.0
             print(f"epoch {epoch:02d} train_loss={mean_loss:.6f}")
             eval_model(model, val_loader, device=device)
         return model
[45]: # number of epochs to train the model
     n = 5
     train(naive_rnn, train_loader, val_loader, n_epochs)
     epoch 01 train_loss=0.606543
     val precision=0.6975 recall=0.8058 f1=0.7477 auc=0.8200
     epoch 02 train_loss=0.417063
     val precision=0.7265 recall=0.8252 f1=0.7727 auc=0.8327
     epoch 03 train_loss=0.305690
     val precision=0.7143 recall=0.8252 f1=0.7658 auc=0.8338
     epoch 04 train_loss=0.203400
     val precision=0.7143 recall=0.7282 f1=0.7212 auc=0.8252
     epoch 05 train_loss=0.125568
     val precision=0.7407 recall=0.7767 f1=0.7583 auc=0.8320
[45]: NaiveRNN(
        (embedding): Embedding(619, 128)
        (gru_fwd): GRU(128, 128, batch_first=True)
        (gru_rev): GRU(128, 128, batch_first=True)
        (fc): Linear(in_features=256, out_features=1, bias=True)
       (sigmoid): Sigmoid()
     )
[46]: '''
     AUTOGRADER CELL. DO NOT MODIFY THIS.
     p, r, f, roc_auc = eval_model(naive_rnn, val_loader)
     print(roc_auc)
     assert roc auc > 0.7, "ROC AUC is too low on the validation set (%f < 0.
      47)"%(roc_auc)
```

val precision=0.7407 recall=0.7767 f1=0.7583 auc=0.8320 0.8320488439595636

```
[47]: '''

AUTOGRADER CELL. DO NOT MODIFY THIS.

'''

[47]: '\nAUTOGRADER CELL. DO NOT MODIFY THIS.\n'

[ ]:
```