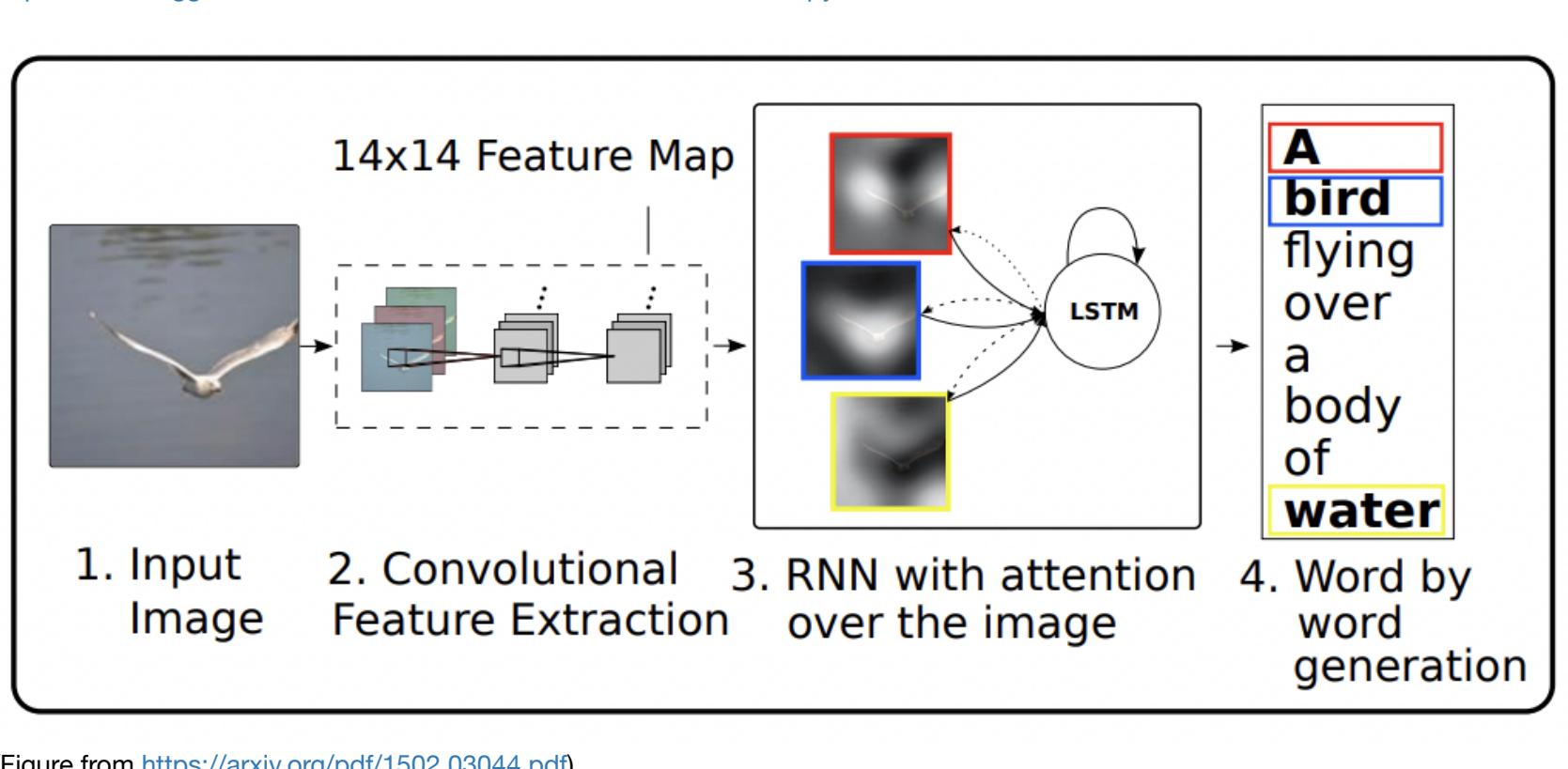
About this notebook

- PyTorch Resnet + LSTM with attention starter code
- Preprocess notebook is here
- Inference notebook is here

If this notebook is helpful, feel free to upvote :)

References

- https://github.com/sgrvinod/a-PyTorch-Tutorial-to-Image-Captioning
- https://github.com/dacon-ai/LG_SMILES_3rd
- https://www.kaggle.com/kaushal2896/bms-mt-show-attend-and-tell-pytorch-baseline



(Figure from https://arxiv.org/pdf/1502.03044.pdf)

Directory settings

In [ ]:
```
# ====================================================
# Directory settings
# ====================================================
import os

OUTPUT_DIR = './'
if not os.path.exists(OUTPUT_DIR):
    os.makedirs(OUTPUT_DIR)
```

Data Loading

In [ ]:
```
import numpy as np
import pandas as pd
import torch

train = pd.read_pickle('../input/inchi-preprocess-2/train2.pkl')

def get_train_file_path(image_id):
    return "../input/bms-molecular-translation/train/{}/{}/{}/{}.png".format(
        image_id[0], image_id[1], image_id[2], image_id
    )

train['file_path'] = train['image_id'].apply(get_train_file_path)

print(f'train.shape: {train.shape}')
display(train.head())
```

In [ ]:
```
class Tokenizer(object):

    def __init__(self):
        self.stoi = {}
        self.itos = {}

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

    def fit_on_texts(self, texts):
        vocab = set()
        for text in texts:
            vocab.update(text.split(' '))
        vocab = sorted(vocab)
        vocab.append('<sos>')
        vocab.append('<eos>')
        vocab.append('<pad>')
        for i, s in enumerate(vocab):
            self.stoi[s] = i
        self.itos = {item[1]: item[0] for item in self.stoi.items()}

    def text_to_sequence(self, text):
        sequence = []
        sequence.append(self.stoi['<sos>'])
        for s in text.split(' '):
            sequence.append(self.stoi[s])
        sequence.append(self.stoi['<eos>'])
        return sequence

    def texts_to_sequences(self, texts):
        sequences = []
        for text in texts:
            sequence = self.text_to_sequence(text)
            sequences.append(sequence)
        return sequences

    def sequence_to_text(self, sequence):
        return ''.join(list(map(lambda i: self.itos[i], sequence)))

    def sequences_to_texts(self, sequences):
        texts = []
        for sequence in sequences:
            text = self.sequence_to_text(sequence)
            texts.append(text)
        return texts

    def predict_caption(self, sequence):
        caption = ''
        for i in sequence:
            if i == self.stoi['<eos>'] or i == self.stoi['<pad>']:
                break
            caption += self.itos[i]
        return caption

    def predict_captions(self, sequences):
        captions = []
        for sequence in sequences:
            caption = self.predict_caption(sequence)
            captions.append(caption)
        return captions

tokenizer = torch.load('../input/inchi-preprocess-2/tokenizer2.pth')
print(f"tokenizer.stoi: {tokenizer.stoi}")
```

In [ ]:
```
train['InChI_length'].max()
```

CFG

In [ ]:
```
# ====================================================
# CFG
# ====================================================
class CFG:
    debug=False
    max_len=275
    print_freq=1000
    num_workers=4
    model_name='resnet34'
    size=224
    scheduler='CosineAnnealingLR' # ['ReduceLROnPlateau', 'CosineAnnealingLR', 'CosineAnnealingWarmRest
arts']
    epochs=1 # not to exceed 9h
    #factor=0.2 # ReduceLROnPlateau
    #patience=4 # ReduceLROnPlateau
    #eps=1e-6 # ReduceLROnPlateau
    T_max=4 # CosineAnnealingLR
    #T_0=4 # CosineAnnealingWarmRestarts
    encoder_lr=1e-4
    decoder_lr=4e-4
    min_lr=1e-6
    batch_size=64
    weight_decay=1e-6
    gradient_accumulation_steps=1
    max_grad_norm=5
    attention_dim=256
    embed_dim=256
    decoder_dim=512
    dropout=0.5
    seed=42
    n_fold=5
    trn_fold=[0] # [0, 1, 2, 3, 4]
    train=True
```

In [ ]:
```
if CFG.debug:
    CFG.epochs = 1
    train = train.sample(n=1000, random_state=CFG.seed).reset_index(drop=True)
```

Library

In [ ]:
```
# ====================================================
# Library
# ====================================================
import sys
sys.path.append('../input/pytorch-image-models/pytorch-image-models-master')

import os
import gc
import re
import math
import time
import random
import shutil
import pickle
from pathlib import Path
from contextlib import contextmanager
from collections import defaultdict, Counter

import scipy as sp
import numpy as np
import pandas as pd
from tqdm.auto import tqdm

import Levenshtein
from sklearn import preprocessing
from sklearn.model_selection import StratifiedKFold, GroupKFold, KFold

from functools import partial

import cv2
from PIL import Image

import torch
import torch.nn as nn
import torch.nn.functional as F
from torch.optim import Adam, SGD
import torchvision.models as models
from torch.nn.parameter import Parameter
from torch.utils.data import DataLoader, Dataset
from torch.nn.utils.rnn import pad_sequence, pack_padded_sequence
from torch.optim.lr_scheduler import CosineAnnealingWarmRestarts, CosineAnnealingLR, ReduceLROnPlateau

from albumentations import (
    Compose, OneOf, Normalize, Resize, RandomResizedCrop, RandomCrop, HorizontalFlip, VerticalFlip,
    RandomBrightness, RandomContrast, RandomBrightnessContrast, Rotate, ShiftScaleRotate, Cutout,
    IAAAdditiveGaussianNoise, Transpose, Blur
    )
from albumentations.pytorch import ToTensorV2
from albumentations import ImageOnlyTransform

import timm

import warnings
warnings.filterwarnings('ignore')

device = torch.device('cuda' if torch.cuda.is_available() else 'cpu')
```

Utils

In [ ]:
```
# ====================================================
# Utils
# ====================================================
def get_score(y_true, y_pred):
    scores = []
    for true, pred in zip(y_true, y_pred):
        score = Levenshtein.distance(true, pred)
        scores.append(score)
    avg_score = np.mean(scores)
    return avg_score


def init_logger(log_file=OUTPUT_DIR+'train.log'):
    from logging import getLogger, INFO, FileHandler,  Formatter,  StreamHandler
    logger = getLogger(__name__)
    logger.setLevel(INFO)
    handler1 = StreamHandler()
    handler1.setFormatter(Formatter("%(message)s"))
    handler2 = FileHandler(filename=log_file)
    handler2.setFormatter(Formatter("%(message)s"))
    logger.addHandler(handler1)
    logger.addHandler(handler2)
    return logger

LOGGER = init_logger()


def seed_torch(seed=42):
    random.seed(seed)
    os.environ['PYTHONHASHSEED'] = str(seed)
    np.random.seed(seed)
    torch.manual_seed(seed)
    torch.cuda.manual_seed(seed)
    torch.backends.cudnn.deterministic = True

seed_torch(seed=CFG.seed)
```

CV split

In [ ]:
```
folds = train.copy()
Fold = StratifiedKFold(n_splits=CFG.n_fold, shuffle=True, random_state=CFG.seed)
for n, (train_index, val_index) in enumerate(Fold.split(folds, folds['InChI_length'])):
    folds.loc[val_index, 'fold'] = int(n)
folds['fold'] = folds['fold'].astype(int)
print(folds.groupby(['fold']).size())
```

Dataset

In [ ]:
```
# ====================================================
# Dataset
# ====================================================
class TrainDataset(Dataset):
    def __init__(self, df, tokenizer, transform=None):
        super().__init__()
        self.df = df
        self.tokenizer = tokenizer
        self.file_paths = df['file_path'].values
        self.labels = df['InChI_text'].values
        self.transform = transform

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

    def __getitem__(self, idx):
        file_path = self.file_paths[idx]
        image = cv2.imread(file_path)
        image = cv2.cvtColor(image, cv2.COLOR_BGR2RGB).astype(np.float32)
        if self.transform:
            augmented = self.transform(image=image)
            image = augmented['image']
        label = self.labels[idx]
        label = self.tokenizer.text_to_sequence(label)
        label_length = len(label)
        label_length = torch.LongTensor([label_length])
        return image, torch.LongTensor(label), label_length


class TestDataset(Dataset):
    def __init__(self, df, transform=None):
        super().__init__()
        self.df = df
        self.file_paths = df['file_path'].values
        self.transform = transform

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

    def __getitem__(self, idx):
        file_path = self.file_paths[idx]
        image = cv2.imread(file_path)
        image = cv2.cvtColor(image, cv2.COLOR_BGR2RGB).astype(np.float32)
        if self.transform:
            augmented = self.transform(image=image)
            image = augmented['image']
        return image
```

In [ ]:
```
def bms_collate(batch):
    imgs, labels, label_lengths = [], [], []
    for data_point in batch:
        imgs.append(data_point[0])
        labels.append(data_point[1])
        label_lengths.append(data_point[2])
    labels = pad_sequence(labels, batch_first=True, padding_value=tokenizer.stoi["<pad>"])
    return torch.stack(imgs), labels, torch.stack(label_lengths).reshape(-1, 1)
```

Transforms

In [ ]:
```
def get_transforms(*, data):

    if data == 'train':
        return Compose([
            Resize(CFG.size, CFG.size),
            Normalize(
                mean=[0.485, 0.456, 0.406],
                std=[0.229, 0.224, 0.225],
            ),
            ToTensorV2(),
        ])

    elif data == 'valid':
        return Compose([
            Resize(CFG.size, CFG.size),
            Normalize(
                mean=[0.485, 0.456, 0.406],
                std=[0.229, 0.224, 0.225],
            ),
            ToTensorV2(),
        ])
```

In [ ]:
```
from matplotlib import pyplot as plt

train_dataset = TrainDataset(train, tokenizer, transform=get_transforms(data='train'))

for i in range(1):
    image, label, label_length = train_dataset[i]
    text = tokenizer.sequence_to_text(label.numpy())
    plt.imshow(image.transpose(0, 1).transpose(1, 2))
    plt.title(f'label: {label}  text: {text}  label_length: {label_length}')
    plt.show()
```

MODEL

In [ ]:
```
class Encoder(nn.Module):
    def __init__(self, model_name='resnet18', pretrained=False):
        super().__init__()
        self.cnn = timm.create_model(model_name, pretrained=pretrained)
        self.n_features = self.cnn.fc.in_features
        self.cnn.global_pool = nn.Identity()
        self.cnn.fc = nn.Identity()

    def forward(self, x):
        bs = x.size(0)
        features = self.cnn(x)
        features = features.permute(0, 2, 3, 1)
        return features
```

In [ ]:
```
class Attention(nn.Module):
    """
    Attention network for calculate attention value
    """
    def __init__(self, encoder_dim, decoder_dim, attention_dim):
        """
        :param encoder_dim: input size of encoder network
        :param decoder_dim: input size of decoder network
        :param attention_dim: input size of attention network
        """
        super(Attention, self).__init__()
        self.encoder_att = nn.Linear(encoder_dim, attention_dim)  # linear layer to transform encoded i
mage
        self.decoder_att = nn.Linear(decoder_dim, attention_dim)  # linear layer to transform decoder's
 output
        self.full_att = nn.Linear(attention_dim, 1)  # linear layer to calculate values to be softmax-e
d
        self.relu = nn.ReLU()
        self.softmax = nn.Softmax(dim=1)  # softmax layer to calculate weights

    def forward(self, encoder_out, decoder_hidden):
        att1 = self.encoder_att(encoder_out)  # (batch_size, num_pixels, attention_dim)
        att2 = self.decoder_att(decoder_hidden)  # (batch_size, attention_dim)
        att = self.full_att(self.relu(att1 + att2.unsqueeze(1))).squeeze(2)  # (batch_size, num_pixels)
        alpha = self.softmax(att)  # (batch_size, num_pixels)
        attention_weighted_encoding = (encoder_out * alpha.unsqueeze(2)).sum(dim=1)  # (batch_size, enc
oder_dim)
        return attention_weighted_encoding, alpha


class DecoderWithAttention(nn.Module):
    """
    Decoder network with attention network used for training
    """

    def __init__(self, attention_dim, embed_dim, decoder_dim, vocab_size, device, encoder_dim=512, drop
out=0.5):
        """
        :param attention_dim: input size of attention network
        :param embed_dim: input size of embedding network
        :param decoder_dim: input size of decoder network
        :param vocab_size: total number of characters used in training
        :param encoder_dim: input size of encoder network
        :param dropout: dropout rate
        """
        super(DecoderWithAttention, self).__init__()
        self.encoder_dim = encoder_dim
        self.attention_dim = attention_dim
        self.embed_dim = embed_dim
        self.decoder_dim = decoder_dim
        self.vocab_size = vocab_size
        self.dropout = dropout
        self.device = device
        self.attention = Attention(encoder_dim, decoder_dim, attention_dim)  # attention network
        self.embedding = nn.Embedding(vocab_size, embed_dim)  # embedding layer
        self.dropout = nn.Dropout(p=self.dropout)
        self.decode_step = nn.LSTMCell(embed_dim + encoder_dim, decoder_dim, bias=True)  # decoding LST
MCell
        self.init_h = nn.Linear(encoder_dim, decoder_dim)  # linear layer to find initial hidden state
 of LSTMCell
        self.init_c = nn.Linear(encoder_dim, decoder_dim)  # linear layer to find initial cell state of
 LSTMCell
        self.f_beta = nn.Linear(decoder_dim, encoder_dim)  # linear layer to create a sigmoid-activated
 gate
        self.sigmoid = nn.Sigmoid()
        self.fc = nn.Linear(decoder_dim, vocab_size)  # linear layer to find scores over vocabulary
        self.init_weights()  # initialize some layers with the uniform distribution

    def init_weights(self):
        self.embedding.weight.data.uniform_(-0.1, 0.1)
        self.fc.bias.data.fill_(0)
        self.fc.weight.data.uniform_(-0.1, 0.1)

    def load_pretrained_embeddings(self, embeddings):
        self.embedding.weight = nn.Parameter(embeddings)

    def fine_tune_embeddings(self, fine_tune=True):
        for p in self.embedding.parameters():
            p.requires_grad = fine_tune

    def init_hidden_state(self, encoder_out):
        mean_encoder_out = encoder_out.mean(dim=1)
        h = self.init_h(mean_encoder_out)  # (batch_size, decoder_dim)
        c = self.init_c(mean_encoder_out)
        return h, c

    def forward(self, encoder_out, encoded_captions, caption_lengths):
        """
        :param encoder_out: output of encoder network
        :param encoded_captions: transformed sequence from character to integer
        :param caption_lengths: length of transformed sequence
        """
        batch_size = encoder_out.size(0)
        encoder_dim = encoder_out.size(-1)
        vocab_size = self.vocab_size
        encoder_out = encoder_out.view(batch_size, -1, encoder_dim)  # (batch_size, num_pixels, encoder
_dim)
        num_pixels = encoder_out.size(1)
        caption_lengths, sort_ind = caption_lengths.squeeze(1).sort(dim=0, descending=True)
        encoder_out = encoder_out[sort_ind]
        encoded_captions = encoded_captions[sort_ind]
        # embedding transformed sequence for vector
        embeddings = self.embedding(encoded_captions)  # (batch_size, max_caption_length, embed_dim)
        # initialize hidden state and cell state of LSTM cell
        h, c = self.init_hidden_state(encoder_out)  # (batch_size, decoder_dim)
        # set decode length by caption length - 1 because of omitting start token
        decode_lengths = (caption_lengths - 1).tolist()
        predictions = torch.zeros(batch_size, max(decode_lengths), vocab_size).to(self.device)
        alphas = torch.zeros(batch_size, max(decode_lengths), num_pixels).to(self.device)
        # predict sequence
        for t in range(max(decode_lengths)):
            batch_size_t = sum([l > t for l in decode_lengths])
            attention_weighted_encoding, alpha = self.attention(encoder_out[:batch_size_t], h[:batch_si
ze_t])
            gate = self.sigmoid(self.f_beta(h[:batch_size_t]))  # gating scalar, (batch_size_t, encoder
_dim)
            attention_weighted_encoding = gate * attention_weighted_encoding
            h, c = self.decode_step(
                torch.cat([embeddings[:batch_size_t, t, :], attention_weighted_encoding], dim=1),
                (h[:batch_size_t], c[:batch_size_t]))  # (batch_size_t, decoder_dim)
            preds = self.fc(self.dropout(h))  # (batch_size_t, vocab_size)
            predictions[:batch_size_t, t, :] = preds
            alphas[:batch_size_t, t, :] = alpha
        return predictions, encoded_captions, decode_lengths, alphas, sort_ind

    def predict(self, encoder_out, decode_lengths, tokenizer):
        batch_size = encoder_out.size(0)
        encoder_dim = encoder_out.size(-1)
        vocab_size = self.vocab_size
        encoder_out = encoder_out.view(batch_size, -1, encoder_dim)  # (batch_size, num_pixels, encoder
_dim)
        num_pixels = encoder_out.size(1)
        # embed start tocken for LSTM input
        start_tockens = torch.ones(batch_size, dtype=torch.long).to(self.device) * tokenizer.stoi["<sos
>"]
        embeddings = self.embedding(start_tockens)
        # initialize hidden state and cell state of LSTM cell
        h, c = self.init_hidden_state(encoder_out)  # (batch_size, decoder_dim)
        predictions = torch.zeros(batch_size, decode_lengths, vocab_size).to(self.device)
        # predict sequence
        for t in range(decode_lengths):
            attention_weighted_encoding, alpha = self.attention(encoder_out, h)
            gate = self.sigmoid(self.f_beta(h))  # gating scalar, (batch_size_t, encoder_dim)
            attention_weighted_encoding = gate * attention_weighted_encoding
            h, c = self.decode_step(
                torch.cat([embeddings, attention_weighted_encoding], dim=1),
                (h, c))  # (batch_size_t, decoder_dim)
            preds = self.fc(self.dropout(h))  # (batch_size_t, vocab_size)
            predictions[:, t, :] = preds
            if np.argmax(preds.detach().cpu().numpy()) == tokenizer.stoi["<eos>"]:
                break
            embeddings = self.embedding(torch.argmax(preds, -1))
        return predictions
```

Helper functions

In [ ]:
```
# ====================================================
# Helper functions
# ====================================================
class AverageMeter(object):
    """Computes and stores the average and current value"""
    def __init__(self):
        self.reset()

    def reset(self):
        self.val = 0
        self.avg = 0
        self.sum = 0
        self.count = 0

    def update(self, val, n=1):
        self.val = val
        self.sum += val * n
        self.count += n
        self.avg = self.sum / self.count


def asMinutes(s):
    m = math.floor(s / 60)
    s -= m * 60
    return '%dm %ds' % (m, s)


def timeSince(since, percent):
    now = time.time()
    s = now - since
    es = s / (percent)
    rs = es - s
    return '%s (remain %s)' % (asMinutes(s), asMinutes(rs))


def train_fn(train_loader, encoder, decoder, criterion,
             encoder_optimizer, decoder_optimizer, epoch,
             encoder_scheduler, decoder_scheduler, device):
    batch_time = AverageMeter()
    data_time = AverageMeter()
    losses = AverageMeter()
    # switch to train mode
    encoder.train()
    decoder.train()
    start = end = time.time()
    global_step = 0
    for step, (images, labels, label_lengths) in enumerate(train_loader):
        # measure data loading time
        data_time.update(time.time() - end)
        images = images.to(device)
        labels = labels.to(device)
        label_lengths = label_lengths.to(device)
        batch_size = images.size(0)
        features = encoder(images)
        predictions, caps_sorted, decode_lengths, alphas, sort_ind = decoder(features, labels, label_le
ngths)
        targets = caps_sorted[:, 1:]
        predictions = pack_padded_sequence(predictions, decode_lengths, batch_first=True).data
        targets = pack_padded_sequence(targets, decode_lengths, batch_first=True).data
        loss = criterion(predictions, targets)
        # record loss
        losses.update(loss.item(), batch_size)
        if CFG.gradient_accumulation_steps > 1:
            loss = loss / CFG.gradient_accumulation_steps
        loss.backward()
        encoder_grad_norm = torch.nn.utils.clip_grad_norm_(encoder.parameters(), CFG.max_grad_norm)
        decoder_grad_norm = torch.nn.utils.clip_grad_norm_(decoder.parameters(), CFG.max_grad_norm)
        if (step + 1) % CFG.gradient_accumulation_steps == 0:
            encoder_optimizer.step()
            decoder_optimizer.step()
            encoder_optimizer.zero_grad()
            decoder_optimizer.zero_grad()
            global_step += 1
        # measure elapsed time
        batch_time.update(time.time() - end)
        end = time.time()
        if step % CFG.print_freq == 0 or step == (len(train_loader)-1):
            print('Epoch: [{0}][{1}/{2}] '
                  'Data {data_time.val:.3f} ({data_time.avg:.3f}) '
                  'Elapsed {remain:s} '
                  'Loss: {loss.val:.4f}({loss.avg:.4f}) '
                  'Encoder Grad: {encoder_grad_norm:.4f}  '
                  'Decoder Grad: {decoder_grad_norm:.4f}  '
                  #'Encoder LR: {encoder_lr:.6f}  '
                  #'Decoder LR: {decoder_lr:.6f}  '
                  .format(
                   epoch+1, step, len(train_loader), batch_time=batch_time,
                   data_time=data_time, loss=losses,
                   remain=timeSince(start, float(step+1)/len(train_loader)),
                   encoder_grad_norm=encoder_grad_norm,
                   decoder_grad_norm=decoder_grad_norm,
                   #encoder_lr=encoder_scheduler.get_lr()[0],
                   #decoder_lr=decoder_scheduler.get_lr()[0],
                   ))
    return losses.avg


def valid_fn(valid_loader, encoder, decoder, tokenizer, criterion, device):
    batch_time = AverageMeter()
    data_time = AverageMeter()
    # switch to evaluation mode
    encoder.eval()
    decoder.eval()
    text_preds = []
    start = end = time.time()
    for step, (images) in enumerate(valid_loader):
        # measure data loading time
        data_time.update(time.time() - end)
        images = images.to(device)
        batch_size = images.size(0)
        with torch.no_grad():
            features = encoder(images)
            predictions = decoder.predict(features, CFG.max_len, tokenizer)
        predicted_sequence = torch.argmax(predictions.detach().cpu(), -1).numpy()
        _text_preds = tokenizer.predict_captions(predicted_sequence)
        text_preds.append(_text_preds)
        # measure elapsed time
        batch_time.update(time.time() - end)
        end = time.time()
        if step % CFG.print_freq == 0 or step == (len(valid_loader)-1):
            print('EVAL: [{0}/{1}] '
                  'Data {data_time.val:.3f} ({data_time.avg:.3f}) '
                  'Elapsed {remain:s} '
                  .format(
                   step, len(valid_loader), batch_time=batch_time,
                   data_time=data_time,
                   remain=timeSince(start, float(step+1)/len(valid_loader)),
                   ))
    text_preds = np.concatenate(text_preds)
    return text_preds
```

Train loop

In [ ]:
```
# ====================================================
# Train loop
# ====================================================
def train_loop(folds, fold):

    LOGGER.info(f"========== fold: {fold} training ==========")

    # ====================================================
    # loader
    # ====================================================
    trn_idx = folds[folds['fold'] != fold].index
    val_idx = folds[folds['fold'] == fold].index

    train_folds = folds.loc[trn_idx].reset_index(drop=True)
    valid_folds = folds.loc[val_idx].reset_index(drop=True)
    valid_labels = valid_folds['InChI'].values

    train_dataset = TrainDataset(train_folds, tokenizer, transform=get_transforms(data='train'))
    valid_dataset = TestDataset(valid_folds, transform=get_transforms(data='valid'))

    train_loader = DataLoader(train_dataset,
                              batch_size=CFG.batch_size,
                              shuffle=True,
                              num_workers=CFG.num_workers,
                              pin_memory=True,
                              drop_last=True,
                              collate_fn=bms_collate)
    valid_loader = DataLoader(valid_dataset,
                              batch_size=CFG.batch_size,
                              shuffle=False,
                              num_workers=CFG.num_workers,
                              pin_memory=True,
                              drop_last=False)

    # ====================================================
    # scheduler
    # ====================================================
    def get_scheduler(optimizer):
        if CFG.scheduler=='ReduceLROnPlateau':
            scheduler = ReduceLROnPlateau(optimizer, mode='min', factor=CFG.factor, patience=CFG.patien
ce, verbose=True, eps=CFG.eps)
        elif CFG.scheduler=='CosineAnnealingLR':
            scheduler = CosineAnnealingLR(optimizer, T_max=CFG.T_max, eta_min=CFG.min_lr, last_epoch=-1
)
        elif CFG.scheduler=='CosineAnnealingWarmRestarts':
            scheduler = CosineAnnealingWarmRestarts(optimizer, T_0=CFG.T_0, T_mult=1, eta_min=CFG.min_l
r, last_epoch=-1)
        return scheduler

    # ====================================================
    # model & optimizer
    # ====================================================
    encoder = Encoder(CFG.model_name, pretrained=True)
    encoder.to(device)
    encoder_optimizer = Adam(encoder.parameters(), lr=CFG.encoder_lr, weight_decay=CFG.weight_decay, am
sgrad=False)
    encoder_scheduler = get_scheduler(encoder_optimizer)

    decoder = DecoderWithAttention(attention_dim=CFG.attention_dim,
                                   embed_dim=CFG.embed_dim,
                                   decoder_dim=CFG.decoder_dim,
                                   vocab_size=len(tokenizer),
                                   dropout=CFG.dropout,
                                   device=device)
    decoder.to(device)
    decoder_optimizer = Adam(decoder.parameters(), lr=CFG.decoder_lr, weight_decay=CFG.weight_decay, am
sgrad=False)
    decoder_scheduler = get_scheduler(decoder_optimizer)

    # ====================================================
    # loop
    # ====================================================
    criterion = nn.CrossEntropyLoss(ignore_index=tokenizer.stoi["<pad>"])

    best_score = np.inf
    best_loss = np.inf

    for epoch in range(CFG.epochs):

        start_time = time.time()

        # train
        avg_loss = train_fn(train_loader, encoder, decoder, criterion,
                            encoder_optimizer, decoder_optimizer, epoch,
                            encoder_scheduler, decoder_scheduler, device)

        # eval
        text_preds = valid_fn(valid_loader, encoder, decoder, tokenizer, criterion, device)
        text_preds = [f"InChI=1S/{text}" for text in text_preds]
        LOGGER.info(f"labels: {valid_labels[:5]}")
        LOGGER.info(f"preds: {text_preds[:5]}")

        # scoring
        score = get_score(valid_labels, text_preds)

        if isinstance(encoder_scheduler, ReduceLROnPlateau):
            encoder_scheduler.step(score)
        elif isinstance(encoder_scheduler, CosineAnnealingLR):
            encoder_scheduler.step()
        elif isinstance(encoder_scheduler, CosineAnnealingWarmRestarts):
            encoder_scheduler.step()

        if isinstance(decoder_scheduler, ReduceLROnPlateau):
            decoder_scheduler.step(score)
        elif isinstance(decoder_scheduler, CosineAnnealingLR):
            decoder_scheduler.step()
        elif isinstance(decoder_scheduler, CosineAnnealingWarmRestarts):
            decoder_scheduler.step()

        elapsed = time.time() - start_time

        LOGGER.info(f'Epoch {epoch+1} - avg_train_loss: {avg_loss:.4f}  time: {elapsed:.0f}s')
        LOGGER.info(f'Epoch {epoch+1} - Score: {score:.4f}')

        if score < best_score:
            best_score = score
            LOGGER.info(f'Epoch {epoch+1} - Save Best Score: {best_score:.4f} Model')
            torch.save({'encoder': encoder.state_dict(),
                        'encoder_optimizer': encoder_optimizer.state_dict(),
                        'encoder_scheduler': encoder_scheduler.state_dict(),
                        'decoder': decoder.state_dict(),
                        'decoder_optimizer': decoder_optimizer.state_dict(),
                        'decoder_scheduler': decoder_scheduler.state_dict(),
                        'text_preds': text_preds,
                       },
                        OUTPUT_DIR+f'{CFG.model_name}_fold{fold}_best.pth')
```

Main

In [ ]:

```
# ====================================================
# main
# ====================================================
def main():

    """
    Prepare: 1.train  2.folds
    """

    if CFG.train:
        # train
        oof_df = pd.DataFrame()
        for fold in range(CFG.n_fold):
            if fold in CFG.trn_fold:
                train_loop(folds, fold)
```

In [ ]:

```
if __name__ == '__main__':
    main()
```