sheet11_main

January 30, 2023

1 Sheet 11

To run in Google Colab (highly recommended for exercise 3) go to: https://colab.research.google.com/drive/1kEEEyD_8uFzl97g7nzeEz5UEBKjpBD48?usp=sharing

1.1 1 Positional Encoding

[ ]:
```
import numpy as np
import matplotlib.pyplot as plt
%matplotlib inline

import torch
import torch.nn as nn
from tqdm.auto import tqdm
```

[ ]:
```
from IPython.display import Image

Image(filename = '1.(a).jpg')
```

[ ]:

(a) Case 1. $K = Q = X + \mathcal{E}$.

score $K^T Q = (X+\mathcal{E})^T (X+\mathcal{E})$

$= (X^T + \mathcal{E}^T)(X+\mathcal{E})$

$= (X^T X + X^T \mathcal{E} + \mathcal{E}^T X + \mathcal{E}^T \mathcal{E})$

$= (X^T X + \mathcal{E}^T \mathcal{E}) + X^T \mathcal{E} + \mathcal{E}^T X$

terms meaning →.

$X^T X$ and $\mathcal{E}^T \mathcal{E}$ → Captures corelations between different features for both feature and positional embedding space.

$\mathcal{E}^T X$ → this matrix calculates projection of each positional embedding vector in the feature space.

$X^T \mathcal{E}$ → this matrix calculates projection of each sample in embedding space.

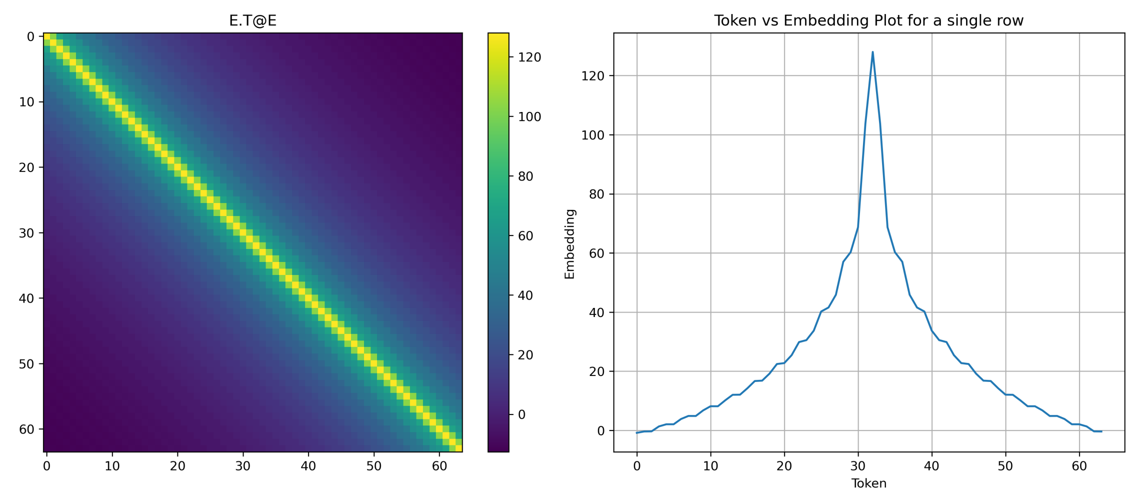
Case 2 →. $K = Q = \text{Cat}(X, \mathcal{E})$.

$K = [\,X \mid \mathcal{E}\,]$

Sort of like additional Samples in features space.

Clearly $K^T Q$ now will be the Matrix which calculates covarience matrix but now with 2N samples.

[ ]:
```
p = 256 # embedding dimension
N = 64  # tokens

E = np.zeros((p,N))

for k in range(int(p/2)):
    for i in range(0,N):
        exp = np.exp(-(k*np.log(10000))/p)
        E[2*k,i] = np.sin(2*i*exp)
        E[2*k+1,i] = np.cos(2*i*exp)

matrix = E.T@E
fig,ax = plt.subplots(1,2,figsize=(16,6),dpi=300)
ax[0].set_title('E.T@E')
im = ax[0].imshow(matrix)
plt.colorbar(im, ax=ax[0],fraction=0.046)

step = np.arange(0,64)
ax[1].plot(step,matrix[32,:])
ax[1].set_xlabel('Token')
ax[1].set_ylabel('Embedding')
ax[1].set_title('Token vs Embedding Plot for a single row')
ax[1].grid()
```

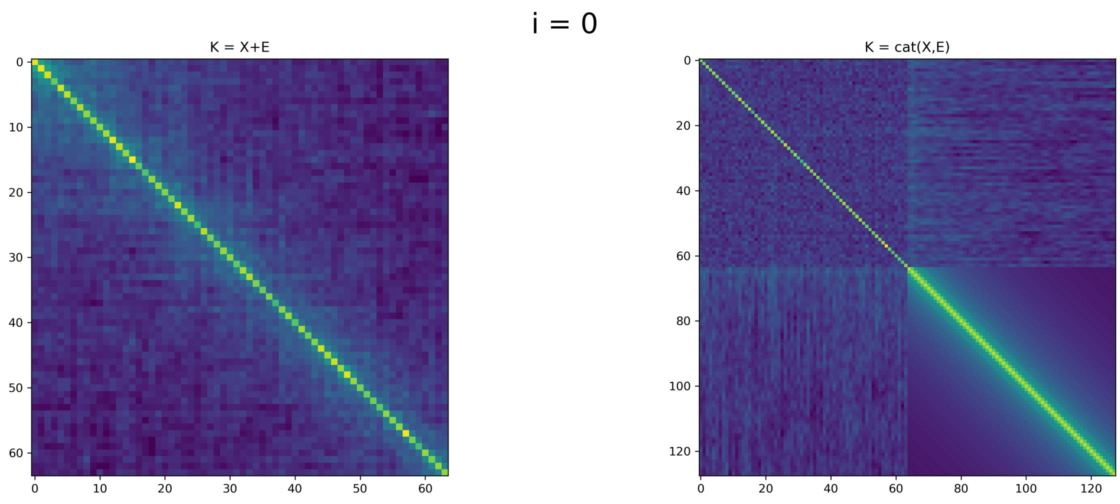


- We see that each embedding dimension is highly correlated with itself, therefore getting the highly dense diagonal.
- As we move away from one dimension to other the covariance oscillates and ‘dies’ exponentially.

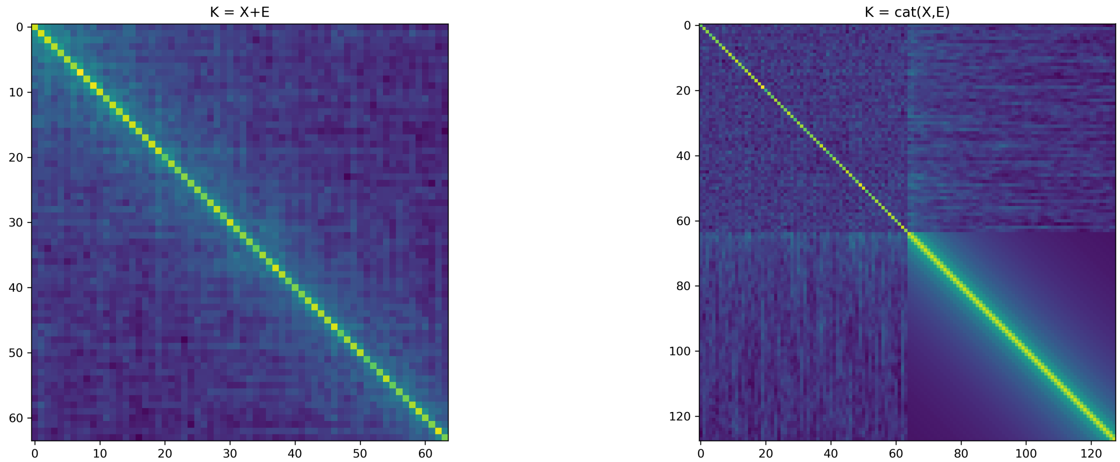
- This means that a particular random feature is correlated to its nearest features locally. As we move away this correlation becomes zero.
- To demonstrate and support our reasoning, we have also plotted a particular row.

1.1.1 1.(C)

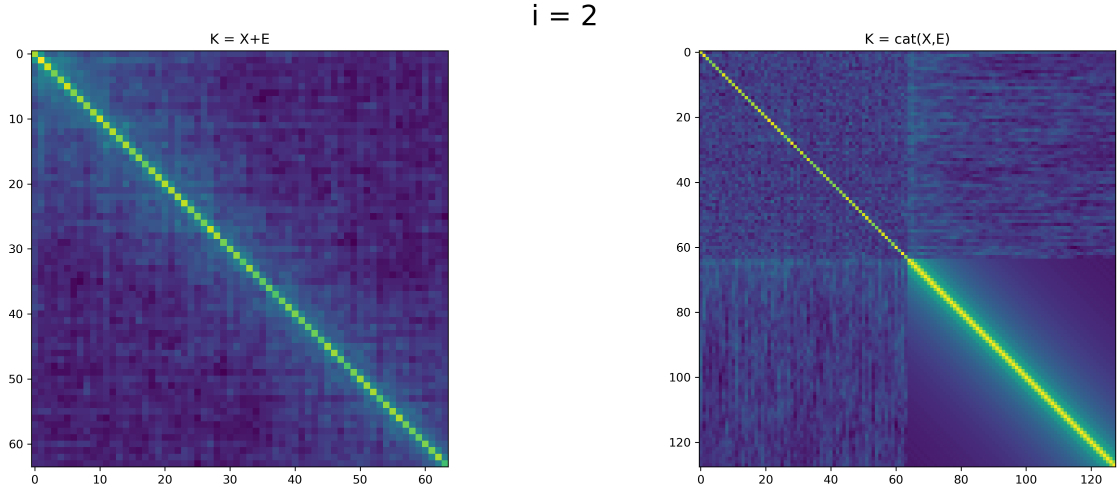
[ ]:
```python
# calculating the variance of E along axis = 1 and taking the average
var = np.mean(np.var(E,axis =1))
mean = np.mean(np.mean(E,axis = 1))

# generating (p X N) elements from a gaussian with different mean and sigma
mu = np.mean(mean)
sigma = np.sqrt(var)


for i in range(5):  ## we will plot the scores for 5 different random features
 ↪which has the same sigma and mean like E
    X = np.random.normal(mu,sigma,size = (p,N))
    K = X + E
    fig,ax = plt.subplots(1,2,figsize=(16,6),dpi=300)
    fig.suptitle(f'{i = }',size=24)
    fig.tight_layout()
    ax[0].imshow(K.T@K)
    ax[0].set_title('K = X+E')

    K = np.hstack((X,E))

    ax[1].set_title('K = cat(X,E)')

    ax[1].imshow(K.T@K)
```



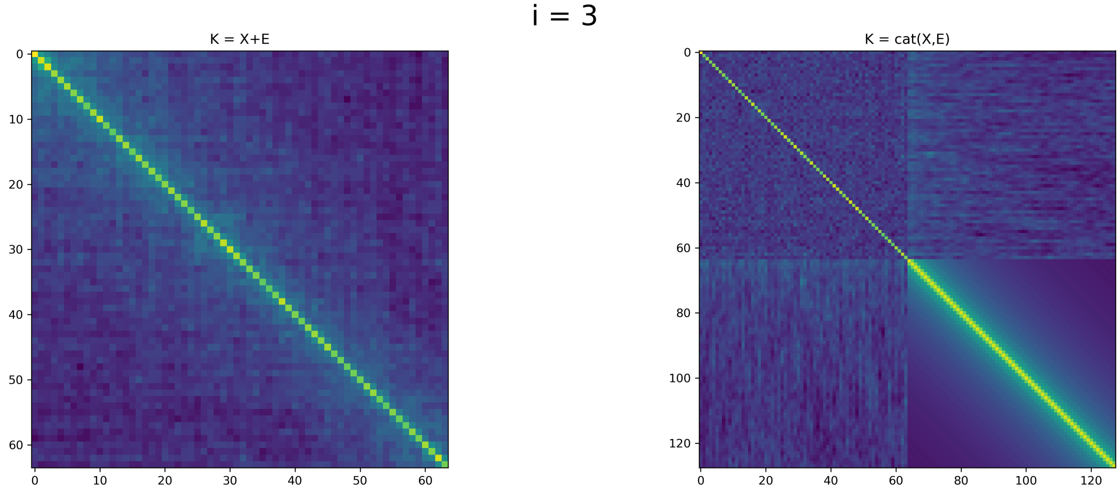
i = 1

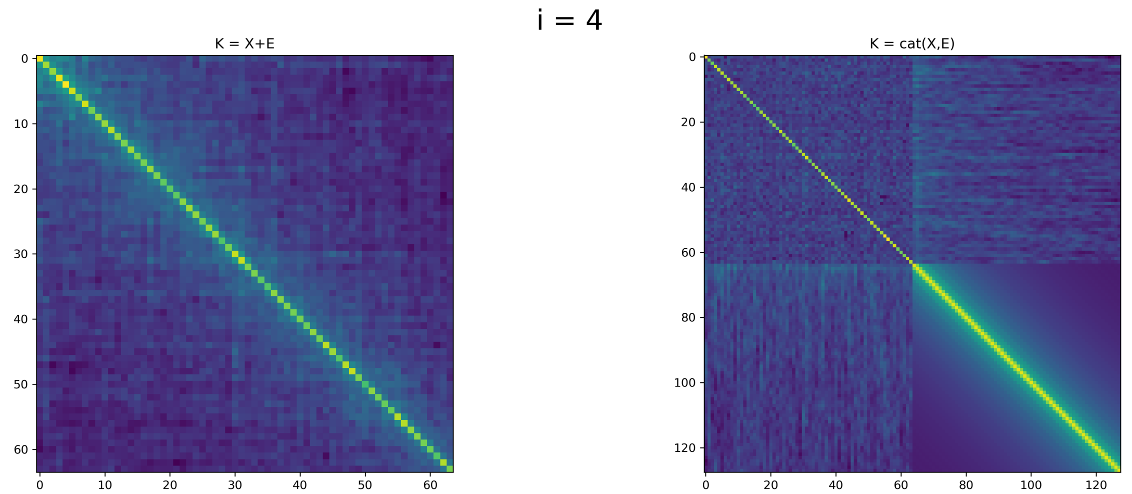


i = 2



i = 3





- We see that for `K = X+E`, the scores peak at the diagonal (same feature) and as we move away from the diagonal (particular feature) covariance is distributed randomly.
- For the concatenated part, `cat(X,E)`, the image is divided into three main parts:
  - The top left and top right parts capture the covariance matrix of the feature and embedding space.
  - Whereas, the off-diagonal part captures covariance between features and embedding space
- We can also say that the `K = (X+E)` part is just the summed version of all constituents part of `cat(X,E)`.

1.2 3 Observing Oversmoothing

[ ]:
```
#@title Install Dependencies and get data from GitHub (will take a few minutes)
# install dependencies
!pip install -q condacolab
import condacolab
condacolab.install()
!conda install mamba -y
!mamba install -c rusty1s -c pytorch -c conda-forge -c lcerrone ctg-benchmark␣
↪cpuonly torchmetrics=0.8.0 jupyter matplotlib

# get data from github
!git clone https://github.com/hci-unihd/mlph_sheet11/
!mv mlph_sheet11/ctg_data .
```

```
[ ]: from ctg_benchmark.loaders.torch_loader import get_cross_validation_loaders,␣
     ↪get_split_loaders
     from ctg_benchmark.evaluation.metrics import NodeClassificationMetrics,␣
     ↪aggregate_class
     import torch
     import numpy as np
     from tqdm import trange
     from tqdm.auto import tqdm
     from torch_geometric.nn.models import GCN
     from torch.optim import Adam
     import torch.nn.functional as F

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

```
cpu
```

```
[ ]: def validation(validation_loader, model):
         # set up evaluation
         eval_metrics = NodeClassificationMetrics(num_classes=9)

         accuracy_records, accuracy_class_records = [], []

         model.eval()
         # TODO: add calculation of mean feature std
         with torch.no_grad():
             val_loss  = 0
             std_batch = 0

             for val_batch in validation_loader:
                 val_batch = val_batch.to(device)
                 pred = model.forward(val_batch.x, val_batch.edge_index)
                 logits = torch.log_softmax(pred, 1)
                 pred = logits.max(1)[1]

                 std_batch += torch.std(logits).item()

                 V_loss_func = F.nll_loss(logits, val_batch.y)
                 val_loss  += V_loss_func.item()
                 # results is a dictionary containing a large number of␣
     ↪classification metrics
                 results = eval_metrics.compute_metrics(pred.cpu(), val_batch.y.
     ↪cpu())
                 acc = results['accuracy_micro']
                 # aggregate class average the single class accuracy and ignores the␣
     ↪embryo sack class (7)
                 acc_class, _ = aggregate_class(results['accuracy_class'], index=7)
```

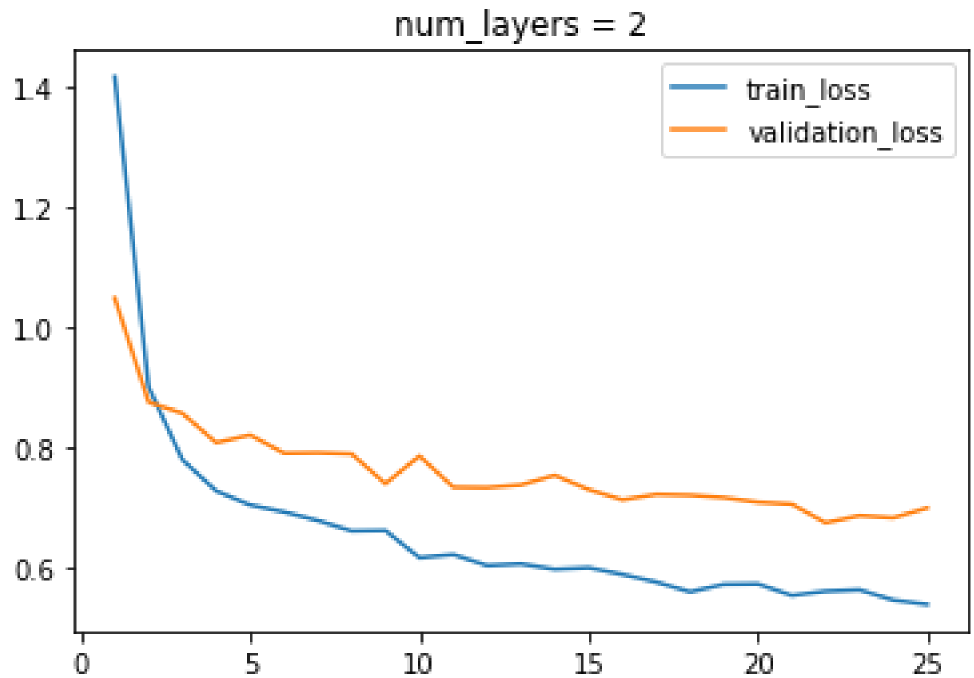
```
            accuracy_records.append(acc)
            accuracy_class_records.append(acc_class)

        val_loss /= len(validation_loader)

        stds = std_batch/len(validation_loader)


    return accuracy_records, accuracy_class_records,val_loss,stds


def simple_trainer(trainer_loader, validation_loader,num_layers=2):

    '''
    We modified this function such that it calls  upper validation function and␣
 ↪returns both train loss

    validation loss

    '''
    model = GCN(in_channels=74, hidden_channels=64, num_layers=num_layers,␣
 ↪out_channels=9, dropout=0.5)
    model = model.to(device)
    optim = Adam(params=model.parameters(), lr=1e-2, weight_decay=1e-5)
    t_range = trange(25, desc=f'Epoch: {0: 03d}, training loss: {0/
 ↪len(trainer_loader): .2f}')
    # basic training loop
    t_loss = []
    v_loss = []
    for epoch in t_range:
        loss_epoch = 0
        for batch in trainer_loader:
            optim.zero_grad()
            batch = batch.to(device)
            pred = model.forward(batch.x, batch.edge_index)
            logits = torch.log_softmax(pred, 1)
            loss = F.nll_loss(logits, batch.y)
            loss.backward()

            optim.step()
            loss_epoch += loss.item()


        t_range.set_description(f'Epoch: {epoch + 1: 03d}, training loss:␣
 ↪{loss_epoch/len(trainer_loader): .2f}')
        t_range.refresh()
```

```
        t_loss.append(loss_epoch/len(trainer_loader))

        a_r,a_c_r,val_loss,stds = validation(validation_loader,model)
        v_loss.append(val_loss)

        ##once the training is done we pass our model to validation and c



    return model,t_loss,v_loss
```

Training GCN with 2 layers

```
[ ]: loaders = get_split_loaders(root='./ctg_data', batch_size=1, shuffle=True,␣
     ↪grs=('label_grs_surface',))
     training_loader, validation_loader = loaders['train'], loaders['val']

     # example training for GCN with 1 layer
     num_layers  = 2
     model,t_loss,v_loss =  simple_trainer(training_loader, validation_loader,␣
     ↪num_layers=num_layers)
     accuracy_records, accuracy_class_records,val_loss,stds =␣
     ↪validation(validation_loader, model)

     # report results
     print(f'\nGCN results for {num_layers=}:')
     print(f'Accuracy {np.mean(accuracy_records):.3f} std: {np.std(accuracy_records):
     ↪.3f}')
     print(f'Class Accuracy {np.mean(accuracy_class_records):.3f} std: {np.
     ↪std(accuracy_class_records):.3f}')


     epoch = np.arange(1,26)
     plt.plot(epoch,t_loss,label = "train_loss")
     plt.plot(epoch,v_loss,label = "validation_loss")
     plt.title("num_layers = "+str(num_layers))
     plt.legend()
     plt.show()
```

```
Epoch:  25, training loss:  0.54: 100%|          | 25/25 [00:21<00:00,
1.15it/s]


GCN results for num_layers=2:
Accuracy 0.749 std: 0.041
Class Accuracy 0.652 std: 0.081
```

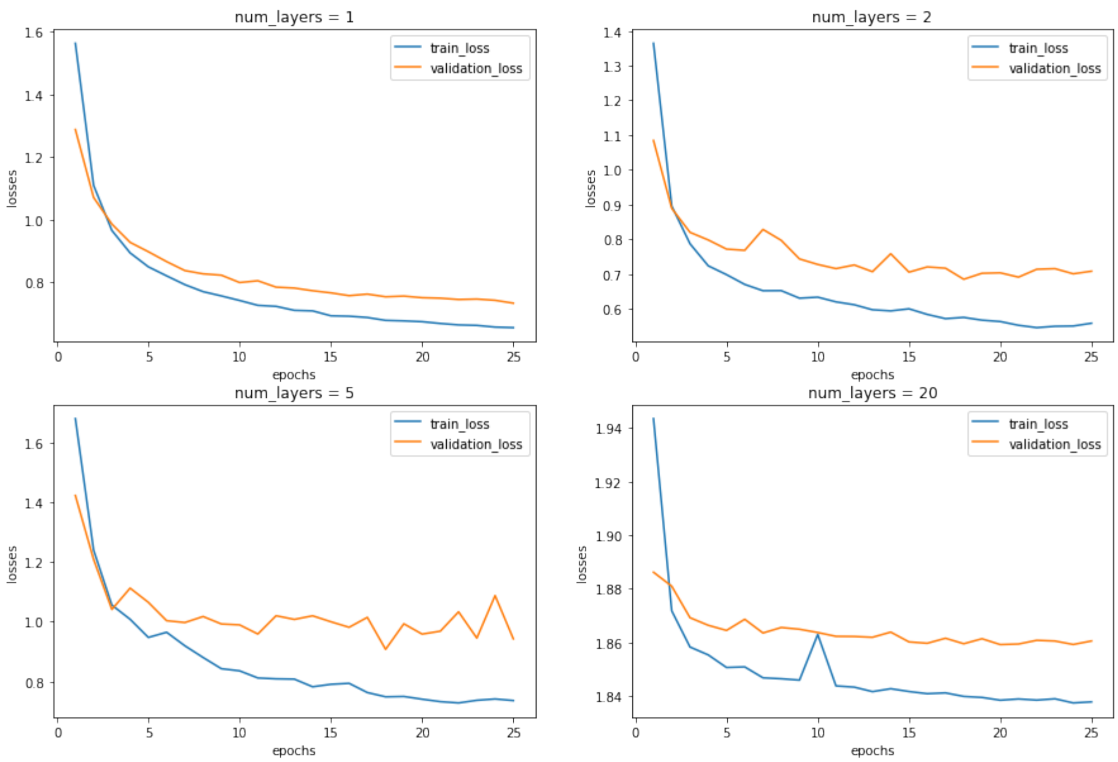


Repeating the same task for num_layers 1,5 and 20

[ ]:
```
epoch = np.arange(1,26)

from matplotlib import pyplot as plt

num_layers_arr = [1,2,5,20]
fig,axs = plt.subplots(2,2,figsize = (15,10))
Models = [model] ##storing

for num_layers,ax in zip(num_layers_arr,axs.flatten()):

    loaders = get_split_loaders(root='./ctg_data', batch_size=1, shuffle=True,␣
 ↪grs=('label_grs_surface',))
    training_loader, validation_loader = loaders['train'], loaders['val']


    model,t_loss,v_loss =  simple_trainer(training_loader, validation_loader,␣
 ↪num_layers=num_layers)
    ax.plot(epoch,t_loss,label = "train_loss")
    ax.plot(epoch,v_loss,label = "validation_loss")
    ax.set_title("num_layers = "+str(num_layers))
    ax.set_xlabel("epochs")
    ax.set_ylabel("losses")
    ax.legend()
```

```
    Models.append(model)
plt.show()
```

```
Epoch:  25, training loss:  0.66: 100%|      | 25/25 [00:10<00:00,
2.34it/s]
Epoch:  25, training loss:  0.56: 100%|      | 25/25 [00:20<00:00,
1.20it/s]
Epoch:  25, training loss:  0.74: 100%|      | 25/25 [00:52<00:00,
2.08s/it]
Epoch:  25, training loss:  1.84: 100%|      | 25/25 [03:19<00:00,
7.98s/it]
```



- In the performance, plots show us that the model with a single layer performs badly as compared to multiple layers.
- We can confirm this by the increment in the validation error as the model progresses through the epochs.
- This is also intuitive as more the no. of layers, better will the model but we also need to take care of efficiency and computation time trade-off.

Computing standard deviations for each for the train models

[ ]:
```python
for num_layers,model in zip(num_layers_arr,Models):
    A,B,V,std = validation(validation_loader,model)

    print(f'{num_layers = }, {std = }')
```

```
num_layers = 1, std = 11.968959728876749
num_layers = 2, std = 4.435128013292949
num_layers = 5, std = 11.36930227279663
num_layers = 20, std = 10.394613981246948
```