# TST base code

May 24, 2023

**TST Representative Code** This is a representative code for developing and training a full-scale encoder-decoder 'Time-Series-Transformer'. Although the architecture is similar to the "Attention is all you need (Vaswani, et. al. 2017) paper, it has to be significantly modified to consider multi-dimensional float-type time-series sequences instead of one-dimensional textual inputs.

```
[]: import numpy as np
from matplotlib import pyplot as plt
import seaborn as sns
import pandas as pd

import torch
import torch.nn as nn
import random
```

How Attention Mechansim Works? Here is a tensorized description of how attention mechanism works along with the shapes of inputs. The output of the block is what you would get out of nn.Multiheadattention block from pytorch.

```
[]: import torch
     import torch.nn as nn
     class Attention(nn.Module):
         def __init__(self, d_model):
             super(Attention, self).__init__()
             self.query = nn.Linear(d_model, d_model)
             self.key = nn.Linear(d model, d model)
             self.value = nn.Linear(d model, d model)
             self.softmax = nn.Softmax(dim=-1)
         def forward(self, x):
             # Compute query, key, and value tensors
             q = self.query(x)
             k = self.key(x)
             v = self.value(x)
             # Compute attention scores
             attn_scores = torch.matmul(q, k.transpose(-2, -1))
             attn_scores = self.softmax(attn_scores)
```

```
# Verify the sum of attention scores
             attn_sum = attn_scores.sum(dim=-1)
             print("Sum of attention scores:", attn_sum)
             # Apply attention weights to values
             attn_output = torch.matmul(attn_scores, v)
             return attn_output, attn_scores
     # Example usage
     batch_size = 1
     seq_length = 12
     d_model = 768
     # Create a random input tensor
     x = torch.randn(batch_size, seq_length, d_model)
     # Create an instance of the Attention module
     attention = Attention(d_model)
     # Pass the input tensor through the attention mechanism
     attn_output, attn_scores = attention(x)
     # Print the shapes of the output tensors
     print("Input shape:", x.shape)
     print("Attention output shape:", attn_output.shape)
     print("Attention scores shape:", attn_scores.shape)
    Sum of attention scores: tensor([[1.0000, 1.0000, 1.0000, 1.0000, 1.0000,
    1.0000, 1.0000, 1.0000, 1.0000,
             1.0000, 1.0000, 1.0000]], grad_fn=<SumBackward1>)
    Input shape: torch.Size([1, 12, 768])
    Attention output shape: torch.Size([1, 12, 768])
    Attention scores shape: torch.Size([1, 12, 12])
    TST Hyperparameters
[]: window_size, prediction_horizon = 12, 6
     chunk_size = int(prediction_horizon/2)
     input_features, output_features = 6, 4
     num_encoder_blocks = 4
     num decoder blocks = 4
     nhead = 8
     dim_FFN = 512 # Dimensions of the FFN inside Encoder/Decoder Blocks
     dropout = 0.1
```

```
d_model = 768 # Vasani (2017)
batch_size = 32
```

### Input Embedding Converting

$$X_{RAW} \rightarrow X_{EM}$$
 
$$[batch_{size}, W, input_{features}] \rightarrow [batch_{size}, W, d_{model}]$$

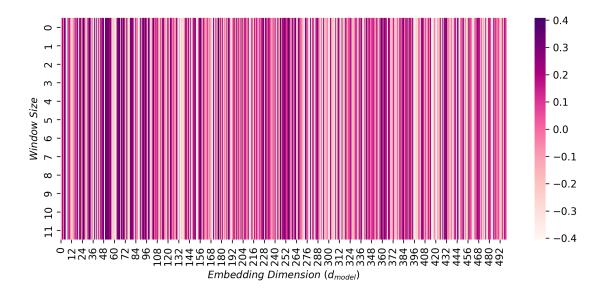
where  $d_{model}$  is the internal dimension of the transformer (lifted states), and W is the window size.

Reference: https://d2l.ai/chapter\_attention-mechanisms-and-transformers/self-attention-and-positional-encoding.html#subsec-cnn-rnn-self-attention

```
class EmbeddingLayer(nn.Module):
    def __init__(self, input_size, d_model):
        super(EmbeddingLayer, self).__init__()
        self.fc = nn.Linear(input_size, d_model)

def forward(self, x):
        x = self.fc(x)
        return x
```

```
[]: # Create a heatmap of the pos_encoded_input tensor
plt.figure(figsize=(10,4), dpi=300)
sns.heatmap(encoded_input[0,:,:500].detach().numpy(), cmap='RdPu')
# plt.xlabel('$Input~Features~(F_{in})$')
plt.xlabel('$Embedding~Dimension~(d_{model})$')
plt.ylabel('$Window~Size$')
# plt.title('Heat Map for Positional Encoding')
plt.show()
```



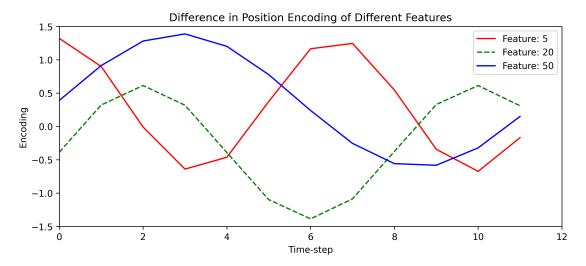
# Positional Encoding Converting

$$X_{EM} \rightarrow X_{PE}$$
 
$$[batch_{size}, W, d_{model}] \rightarrow [batch_{size}, W, d_{model}]$$

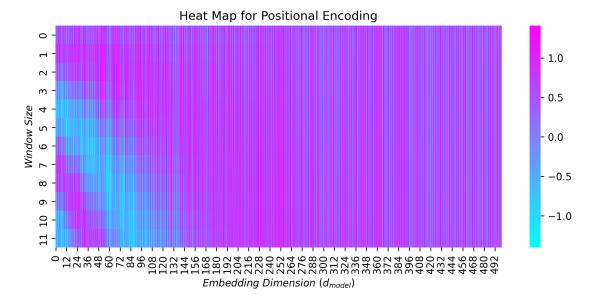
```
[]: class PositionalEncoding(nn.Module): #@save
         """Positional encoding."""
         def __init__(self, d_model, dropout, max_len=1000):
             super().__init__()
             self.dropout = nn.Dropout(dropout)
             # Create a long enough P
             self.P = torch.zeros((1, max_len, d_model))
            position = torch.arange(max_len, dtype=torch.float32).reshape(-1, 1)
             div_term = torch.pow(10000, torch.arange(0, d_model, 2, dtype=torch.
      →float32) / d_model)
            X = position/div_term
             # X = torch.arange(max_len, dtype=torch.float32).reshape(
                   -1, 1) / torch.pow(10000, torch.arange(
                   0, d_model, 2, dtype=torch.float32) / d_model)
             self.P[:, :, 0::2] = torch.sin(X)
             self.P[:, :, 1::2] = torch.cos(X)
         def forward(self, X):
            X = X + self.P[:, :X.shape[1], :].to(X.device)
            return self.dropout(X)
```

Visual representation of positional encoding of different features

```
[]: # Define the colors and linestyles for each line
     colors = ['red', 'green', 'blue']
     linestyles = ['-', '--', '-']
     # Plot each line with a different color and linestyle
     plt.figure(figsize=(10,4), dpi=300)
     for i, color, linestyle in zip([5, 20, 50], colors, linestyles):
         plt.plot(torch.arange(window_size), pos_encoded_input[0, :, i].detach(),__
      ⇔color=color, linestyle=linestyle, label=f'Feature: {i}')
     plt.legend()
     # Set the x-axis and y-axis limits
     plt.xlim(0, window_size)
     plt.ylim([-1.5,1.5])
     plt.title('Difference in Position Encoding of Different Features')
     plt.ylabel('Encoding')
     plt.xlabel('Time-step')
     plt.show()
```



```
[]: # Create a heatmap of the pos_encoded_input tensor
plt.figure(figsize=(10,4), dpi=300)
sns.heatmap(pos_encoded_input[0,:,:500].detach().numpy(), cmap='cool')
plt.xlabel('$Embedding~Dimension~(d_{model})$')
plt.ylabel('$Window~Size$')
plt.title('Heat Map for Positional Encoding')
plt.show()
```



### **Encoder Block**

# 1. General Instructions:

Converting

$$X_{PE} \rightarrow X_{EN_i}$$
 [for  $i = 1$ ]

$$X_{EN_{i-1}} \rightarrow X_{EN_i} \ [for i \neq 1]$$

Dimensions:

$$[batch_{size}, W, d_{model}] \rightarrow [batch_{size}, W, d_{model}]$$

where i is the  $i^{th}$  encoder block.

- 2. **Layernorm:** LayerNorm  $(d_{model})$  normalizes the input  $[batch_{size}, W, d_{model}]$  in the  $d_{model}$  dimension to give out an output of the same dimensions  $[batch_{size}, W, d_{model}]$ .
- 3. Output of 'N' Encoder Blocks:

Any layer in the Transformer encoder does not change the shape of the input vectors. The positionally encoded input has the dimensions  $[batch_{size}, W, d_{model}]$ , and the output from all the encoded blocks has the dimension  $[batch_{size}, W, d_{model}]$ .

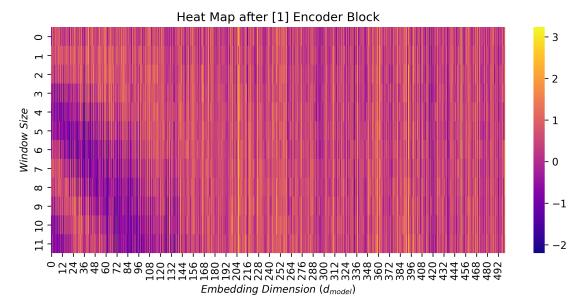
```
[]: class TransformerEncoderBlock(nn.Module):
         """The Transformer encoder block."""
         def __init__(self, d_model, nhead, dim_feedforward, dropout):
             super().__init__()
             self.self_attn = nn.MultiheadAttention(d_model, nhead,__
      →dropout=dropout,batch_first=True)
             self.feedforward = nn.Sequential(
                 nn.Linear(d_model, dim_feedforward),
                 nn.ReLU(),
                 nn.Dropout(p=dropout),
                 nn.Linear(dim feedforward, d model),
                 nn.Dropout(p=dropout)
             )
             self.norm1 = nn.LayerNorm(d_model)
             self.norm2 = nn.LayerNorm(d_model)
             self.dropout1 = nn.Dropout(p=dropout)
             self.dropout2 = nn.Dropout(p=dropout)
         def forward(self, x):
             residual = x
             x = self.norm1(x)
             x, _ = self.self_attn(x, x, x)
             x = self.dropout1(x)
             x = residual + x
             residual = x
             x = self.norm2(x)
             x = self.feedforward(x)
             x = self.dropout2(x)
             x = residual + x
             return x
[]: encoder_block =_
     output = encoder_block(pos_encoded_input)
     print('Encoder Output [batch_size, window_size, d_model]:\n',output.shape)
```

```
-TransformerEncoderBlock(d_model,nhead=nhead,dim_feedforward=dim_FFN,dropout=dropout)
```

```
Encoder Output [batch_size, window_size, d_model]:
 torch.Size([32, 12, 768])
```

Visualize the 'transformation' on the 'positonally encoded input' after an 'Encoder Block'

```
[]: # Create a heatmap of the pos_encoded_input tensor
plt.figure(figsize=(10,4), dpi=300)
sns.heatmap(output[0,:,:500].detach().numpy(), cmap='plasma')
plt.xlabel('$Embedding~Dimension~(d_{model})$')
plt.ylabel('$Window~Size$')
plt.title('Heat Map after [1] Encoder Block')
plt.show()
```

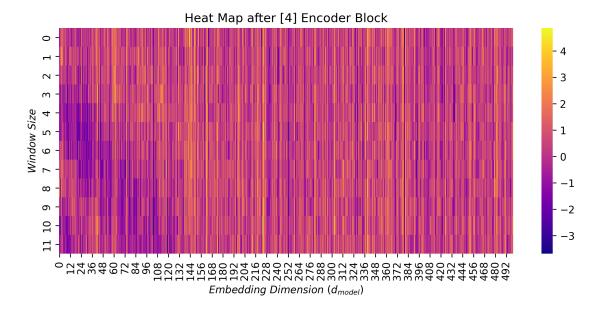


# Stacking Multiple Encoder Blocks

```
x = self.pos_encoder(x) # Add positional encoding
for block in self.encoder_blocks:
    x = block(x) # Pass through the encoder TSTBlock modules
return x
```

Visualizing Output from Multiple Encoded Blocks

Shape after Multiple Encoder Blocks: torch.Size([32, 12, 768])



### Decoder Block

# 1. General Instructions:

Converting

$$X_{EN_i} \rightarrow X_{DEC_1}$$
 [for  $i = 1$ ]  
 $X_{DEC_{i-1}} \rightarrow X_{DEC_{i}}$  [for  $i \neq 1$ ]

Dimensions:

$$[batch_{size}, W, d_{model}] \rightarrow [batch_{size}, H + \lambda, d_{model}]$$

where W is the window size (used in the encoder side of things), and H is the prediction horizon (used in the decoder side of things).

### 2. Decoder Linear Layer and Positional Encoding

The decoder embedding layer takes in the input  $(y_{raw})$  that has dimensions  $[batch_{size}, H, F_{out}]$  \$, and converts it to  $[batch_{size}, H, d_{model}]$  represented by  $Y_{EM}$  The positional encoder for the decoder side uses positional encoding with  $max_{len} = (H + chunk_{size})$  to convert it to  $Y_{PE}$ .

### 3. Output of 'M' Decoder Blocks:

The decoder takes in  $(y_{raw})$  of size  $[batch_{size}, H, F_{out}]$  and converts it to a decoder output of size  $[batch_{size}, H, d_{model}]$ .

#### 4. **Note:**

The internal dimension of the transformer  $(d_{model})$  should be the same for the encoder and decoder side. However, on encoder side the 'seq\_len' is W, and on the decoder side it is H.\*

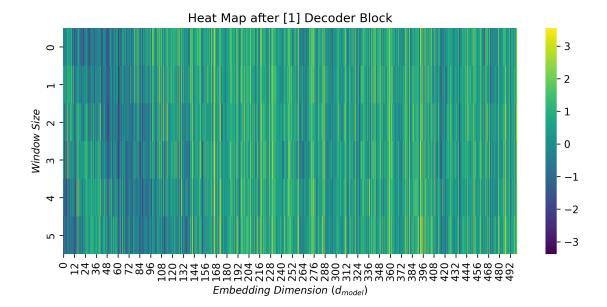
```
[]: class TransformerDecoderBlock(nn.Module): #@save
         """The Transformer Decoder Block."""
         def __init__(self, d_model, nhead, dim_feedforward, dropout):
             super().__init__()
             self.self_attn = nn.MultiheadAttention(d_model, nhead,__
      →dropout=dropout,batch_first=True)
             self.cross_attn = nn.MultiheadAttention(d_model, nhead,_
      →dropout=dropout,batch_first=True)
             self.feedforward = nn.Sequential(
                 nn.Linear(d_model, dim_feedforward),
                 nn.ReLU(),
                 nn.Dropout(p=dropout),
                 nn.Linear(dim_feedforward, d_model),
                 nn.Dropout(p=dropout)
             )
             self.norm1 = nn.LayerNorm(d_model)
             self.norm2 = nn.LayerNorm(d_model)
             self.norm3 = nn.LayerNorm(d_model)
             self.dropout1 = nn.Dropout(p=dropout)
```

```
self.dropout2 = nn.Dropout(p=dropout)
             self.dropout3 = nn.Dropout(p=dropout)
         def forward(self, x, memory):
             residual = x
             x = self.norm1(x)
             x, _ = self.self_attn(x, x, x)
             x = self.dropout1(x)
             x = residual + x
             residual = x
             x = self.norm2(x)
             x, cross_attn_weights = self.cross_attn(x, memory, memory)
             x = self.dropout2(x)
             x = residual + x
             residual = x
             x = self.norm3(x)
             x = self.feedforward(x)
             x = self.dropout3(x)
             x = residual + x
             return x, cross_attn_weights
[]: sample_decoder = torch.zeros(batch_size, prediction_horizon, d_model)
     decoder_block=_
      TransformerDecoderBlock(d_model,nhead=nhead,dim_feedforward=dim_FFN,dropout=dropout)
     # decoded_output = decoder_block(output[:,-prediction_horizon:,:
      →], sample decoder)
     decoded_output, cross attn_weights = decoder_block(output[:,-prediction_horizon:

¬,:],output[:,-prediction_horizon:,:])
     print('Decoder Output [batch_size, prediction_horizon, d_model]:

¬\n',decoded_output.shape)
     # Create a heatmap
     plt.figure(figsize=(10,4), dpi=300)
     sns.heatmap(decoded output[0,:,:500].detach().numpy(), cmap='viridis')
     plt.xlabel('$Embedding~Dimension~(d_{model})$')
     plt.ylabel('$Window~Size$')
     plt.title('Heat Map after [1] Decoder Block')
    plt.show()
    Decoder Output [batch_size, prediction_horizon, d_model]:
```

torch.Size([32, 6, 768])



# Stacking Multiple Decoder Blocks

```
[]: class Multiple_Decoders(nn.Module):
        def __init__(self, input_size, output_size, d_model, nhead,__
      dim_feedforward, num_decoder_blocks, w, h, chunk_size, dropout):
             super(Multiple_Decoders, self).__init__()
             self.w = w
             self.h = h
             self.decoder_blocks = nn.ModuleList([TransformerDecoderBlock(d_model,_
      →nhead, dim_feedforward,dropout=dropout) for _ in range(num_decoder_blocks)])
             self.cross_attn_weights = [] # List to store cross-attention weights
             self.decoder_linear = EmbeddingLayer(output_size, d_model)
             self.pos_decoder = PositionalEncoding(d_model,max_len = self.h +__
      ⇔chunk_size,dropout=dropout)
        def forward(self, x, memory):
            x = self.decoder_linear(x) # Pass through the encoder linear layer
             x = self.pos_decoder(x) # Add positional encoding
             for block in self.decoder_blocks:
                 x, cross_attn_weights = block(x, memory) # Pass through the
      ⇔decoder TSTBlock modules
                 self.cross_attn_weights.append(cross_attn_weights) # Save the_
      ⇔cross-attention weights
```

#### return x

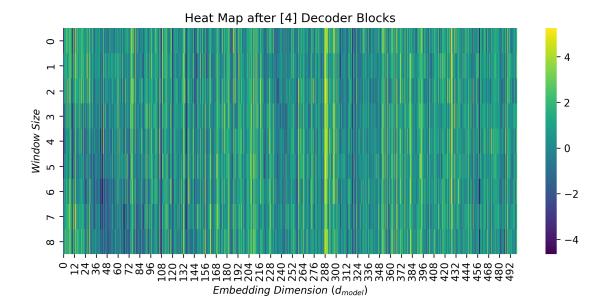
Visualizing output from just the decoder:

First we need to take  $X_{RAW}$  and then run it through the encoder blocks, and then combine  $y_{RAW}$  for the cross-attention.

```
[]: sample_decoder = torch.zeros(batch_size, chunk_size+prediction_horizon,_
      →output_features)
     multiple_encoder_blocks =_u
      -Multiple_Encoders(input_size=input_features,output_size=output_features,
      →d_model=d_model,nhead=nhead,dim_feedforward=dim_FFN
                                        ,num_encoder_blocks=num_encoder_blocks,
                                        w=window_size,h=prediction_horizon,
                                        dropout=dropout)
     encoder_output = multiple_encoder_blocks(sample)
     print('Shape after Multiple Encoder Blocks:', encoder_output.shape)
     multiple_decoder_blocks = Multiple_Decoders(input_size=input_features,_
      ⇔output_size=output_features,
      ⇒d model=d model,nhead=nhead,dim feedforward=dim FFN,

¬num_decoder_blocks=num_decoder_blocks,
                                                 w=window_size,h=prediction_horizon,u
      ⇔chunk_size=chunk_size,
                                                 dropout=dropout)
     decoder_output = multiple_decoder_blocks(sample_decoder,encoder_output[:
      -, -(chunk_size+prediction_horizon):,:])
     attention_weights = multiple_decoder_blocks.cross_attn_weights
     # Create a heatmap of the pos_encoded_input tensor
     plt.figure(figsize=(10,4), dpi=300)
     sns.heatmap(decoder_output[0,:,:500].detach().numpy(), cmap='viridis')
     plt.xlabel('$Embedding~Dimension~(d_{model})$')
     plt.ylabel('$Window~Size$')
     plt.title('Heat Map after [' + str(num_decoder_blocks) + '] Decoder Blocks')
     plt.show()
```

Shape after Multiple Encoder Blocks: torch.Size([32, 12, 768])



Visualizing attention weights from multiple decoders

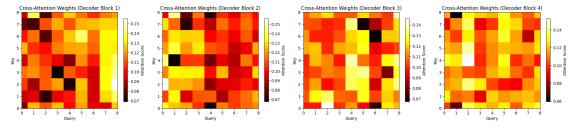
```
[]: batch_index = random.randint(0, batch_size - 1)
     num_blocks = len(attention_weights)
     # Create a single figure with subplots
     fig, axes = plt.subplots(1, num_blocks, figsize=(num_blocks * 5,10))
     # Generate an array of alpha values
     alpha_array = np.linspace(0.4, 1, num_blocks)
     # Iterate over the attention weights and plot them
     for i, weights in enumerate(attention_weights):
         # Select the attention weights for the specified batch
         weights = weights[batch_index, :, :]
         # Select the corresponding subplot
         ax = axes[i]
         # Plot the attention weights with the specified alpha value
         img = ax.imshow(weights.squeeze(0).detach().numpy(), cmap='hot',__
      →interpolation='nearest')
         ax.set_title('Cross-Attention Weights (Decoder Block {})'.format(i + 1))
         ax.set_xlabel('Query')
         ax.set_ylabel('Key')
         # Set xlim and ylim to match weights.shape[-1]
         xlim = weights.shape[-1]
```

```
ylim = weights.shape[-1]
ax.set_xlim(1, xlim-1)
ax.set_ylim(1, ylim-1)

# Set xticks and yticks to display exact integers
ax.set_xticks(np.arange(0, xlim, 1))
ax.set_yticks(np.arange(0, ylim, 1))

# Add a color bar to the subplot
cbar = fig.colorbar(img, ax=ax, shrink=0.3)
cbar.ax.set_ylabel('Attention Score')

plt.tight_layout()
plt.show()
```



# **Output Module**

#### 1. General Instructions:

Converting decoder output to the model predictions  $(y_{tgt})$  of dimensions  $[batch_{size}, H + \lambda, F_{out}]$ .

#### 1. Entire Chain of Conversions for TSTs:

$$\begin{split} X_{RAW} &\to X_{EM} \\ X_{EM} &\to X_{PE} \\ X_{PE} &\to X_{EN_i} \\ X_{EN_i} &\to Y_{DEC_j} \\ Y_{DEC_i} &\to Y_{tqt} \end{split}$$

## 2. Dimensions:

The encoder embedding layer takes in input  $(X_{RAW})$  that has dimensions  $[batch_{size}, W, F_{in}]$ , and converts it to  $[batch_{size}, W, d_model]$  represented by  $X_{EM}$  The positional encoder for the decoder side uses positional encoding with  $max\_len = W$  to convert it to  $X_{PE}$ . Then,  $X_{PE}$  is converted to  $X_{EN}$ , through encoder blocks.

The decoder embedding layer takes in input  $(y_{raw})$  that has dimensions  $[batch_{size}, H+, F_{out}]$ , and converts it to  $[batch_{size}, H+\lambda, d_{m}odel]$  represented by

 $Y_{EM}$  The positional encoder for the decoder side uses positional encoding with  $max\_len = (H+chunk\_size)$  to convert it to  $Y_{PE}$ . The the decoder blocks convert this to a tensor of dimensions  $[batch_{size}, H + \lambda, d_{model}]$ .

Finally,  $[batch_{size}, H + \lambda, d_{model}]$  is converted to  $[batch_{size}, H, F_{out}]$  (model predictions).

```
[]: output_FFN = EmbeddingLayer(d_model,output_features)
    final_output = output_FFN(decoder_output)
    final_output = final_output[:,-prediction_horizon:,:]

print('Decoder Output: ', decoder_output.shape)
print("Final Output: ", final_output.shape)
```

Decoder Output: torch.Size([32, 9, 768])
Final Output: torch.Size([32, 6, 4])

### 0.0.1 Combining all the modules for making a TST

```
[]: class TimeSeriesTransformer(nn.Module):
         def __init__(self, input_size, output_size, d_model=768, nhead=8,_
      ⇒dim feedforward=512,
                      num_encoder_blocks=6, num_decoder_blocks=6,
                      dropout=0.1,
                      window_size=window_size,_
      aprediction_horizon=prediction_horizon, chunk_size = chunk_size):
             super(TimeSeriesTransformer, self).__init__()
             # Set the model parameters
             self.d_model = d_model
             self.nhead = nhead
             self.num_encoder_blocks = num_encoder_blocks
             self.num_decoder_blocks = num_decoder_blocks
             self.window_size = window_size
             self.prediction_horizon = prediction_horizon
             # Encoder blocks
             self.multiple_encoder_blocks =_u
      -Multiple_Encoders(input_size=input_features,output_size=output_features,
      →d_model=d_model,nhead=nhead,dim_feedforward=dim_FFN
                                         ,num_encoder_blocks=num_encoder_blocks,
                                        w=window_size,h=prediction_horizon,
                                        dropout=dropout)
             # Decoder blocks
             self.multiple_decoder_blocks =_u
      Multiple_Decoders(input_size=input_features, output_size=output_features,
```

```
d_model=d_model,nhead=nhead,dim_feedforward=dim_FFN,
⇒num decoder blocks=num decoder blocks,
                                        w=window_size,h=prediction_horizon,u
⇔chunk_size=chunk_size,
                                        dropout=dropout)
      # Output layer
      self.output_FFN = EmbeddingLayer(d_model,output_features)
  def forward(self, x_enc, x_dec):
      # Encode the input time series data
      encoder_output = self.multiple_encoder_blocks(x_enc)
      # Decode the input time series data
      decoder_output = self.multiple_decoder_blocks(x_dec, encoder_output[:,u
# Pass the decoded output through the output layer
      final_output = self.output_FFN(decoder_output)
      # Return only the predicted values
      # final_output = final_output[:, -prediction_horizon:, :]
      return final_output
```

Testing if the Entire TST Block works

```
TST_output = model(input_sample,output_sample)
print(TST_output.shape)
```

```
Encoder Input Dimensions: torch.Size([32, 12, 6])
Decoder Input Dimensions: torch.Size([32, 6, 4])
TST Output Dimensions: torch.Size([32, 6, 4])
torch.Size([32, 6, 4])
```

### 0.0.2 Training Module for TST

Code snippet for training a TST from scratch given a train\_loader, and val\_loader dataset can be imported/generated.

```
[]: def train_model(model, train_loader, val_loader, loss_fn, optimizer, scheduler,__
      →num_epochs):
        train_losses = [] # List to store training losses for each epoch
        val_losses = [] # List to store validation losses for each epoch
        for epoch in range(num_epochs):
             # Training
            model.train() # Set the model to training mode
            train_loss = 0.0
             for i, (x_enc, x_dec, y) in enumerate(train_loader):
                 optimizer.zero_grad() # Clear the gradients
                 output = model(x_enc, x_dec) # Forward pass
                 loss = loss_fn(output, y) # Compute the loss
                 loss.backward() # Backward pass
                 optimizer.step() # Update the model's parameters
                 train_loss += loss.item() # Accumulate the training loss for the
      ⇔current batch
             scheduler.step() # Update the learning rate scheduler
             avg_train_loss = train_loss / len(train_loader) # Calculate the_
      →average training loss for the epoch
            train_losses.append(avg_train_loss) # Store the average training loss
             # Validation
            model.eval() # Set the model to evaluation mode
            val_loss = 0.0
            with torch.no_grad():
                 for i, (x_enc, x_dec, y) in enumerate(val_loader):
                     output = model(x_enc, x_dec) # Forward pass (no gradients_
      \rightarrowneeded)
                     loss = loss_fn(output, y) # Compute the loss
                     val_loss += loss.item() # Accumulate the validation loss for_
      ⇒the current batch
                 avg_val_loss = val_loss / len(val_loader) # Calculate the average_u
      ⇔validation loss for the epoch
```

```
val_losses.append(avg_val_loss) # Store the average validation loss

# Print the epoch number and the corresponding training and validation

$\times\losses$

print(f"Epoch {epoch+1}/{num_epochs}, train loss: {avg_train_loss:.4f}, \to

$\times\losses$ {avg_val_loss:.4f}")

return train_losses, val_losses # Return the training and validation

$\times\losses for all epochs$
```