Data Preprocessing

In [1]:
```python
import pandas as pd
import numpy as np
import os
from sklearn.preprocessing import StandardScaler
from sklearn.model_selection import train_test_split
```

In [2]:
```python
def get_csv_files(target_dir):
    """Returns a list of all CSV file paths in the specified directory."""
    return [os.path.join(target_dir, f) for f in os.listdir(target_dir) if f.endswith('.csv')]

def save_plot(file_name, dir_path, plt):
    """Save the given plot to the specified directory."""

    # Construct the full path for the image
    full_path = os.path.join(dir_path, file_name)

    # Save the plot
    plt.savefig(full_path)

    # Print a message indicating the image has been saved
    print(f"Image has been saved at {full_path}")
```

In [3]:
```python
# Constants
DTYPES = {"cashier": "object", "routing_no": "object", "tm_disc": "object"}
DROP_COLS = ["rcpt_id", 'tndr_acct', 'routing_no', 'start_tm', 'end_tm', 'sls_d', 'crt_whl_a']
FLAG_COLS = ['gc_flg', 'prc_ovrd_exc_flg', 'void_flag', 'tm_flg']
FLAG_REPLACE = {'Y': 1, '': 0, ' ': 0}
```

In [4]:
```python
Image_Folder = 'Images'
Model_Folder = 'models'
Result_Folder = 'Results'
Data_Folder = 'data'
Data_SubFolder = 'Target_Data\Receipts_2'
SubFolder = "All_Purchases"

data_dir_path = os.path.join(Data_Folder, Data_SubFolder)

image_dir_path = os.path.join(Image_Folder, SubFolder)
os.makedirs(image_dir_path, exist_ok=True)

model_dir_path = os.path.join(Model_Folder, SubFolder)
os.makedirs(model_dir_path, exist_ok=True)

result_dir_path = os.path.join(Result_Folder, SubFolder)
os.makedirs(result_dir_path, exist_ok=True)
```

In [5]:
```python
# Get CSV files
csv_files = get_csv_files(data_dir_path)

# Import and concatenate CSV files
dfs = [pd.read_csv(file, dtype=DTYPES) for file in csv_files]
df = pd.concat(dfs, ignore_index=True)

# Backup original dataframe
df_orig = df.copy().reset_index(drop=True)
```

In [6]:
```
# Manipulate the 'register_i' column
df['register_i'] = df['rcpt_id'].str.split('-').str[2].str.lstrip('0')
df['register_i'] = df['register_i'].replace('', 'Unknown').fillna('Unknown')

# Convert columns to binary representations
df['guest_profile_id'] = df['guest_profile_id'].notna().astype(int)
df['circle_id'] = df['circle_id'].notna().astype(int)

# Update FLAG_COLS and other columns
df = (df.fillna({col: 0 for col in FLAG_COLS})
      .replace({col: FLAG_REPLACE for col in FLAG_COLS})
      .astype({col: int for col in FLAG_COLS})
      .assign(tndr_type=lambda x: x['tndr_type'].str.strip(),
              sls_d=lambda x: pd.to_datetime(x['sls_d'], format='%Y-%m-%d'),
              start_tm=lambda x: pd.to_datetime(x['sls_d'].dt.date.astype(str) + ' ' + x['start_tm'].astype(str))
      .reset_index(drop=True)))

# Extract date and time features
df['year'] = df['start_tm'].dt.year
df['month'] = df['start_tm'].dt.month
df['hour'] = df['start_tm'].dt.hour
df['day_of_year'] = df['start_tm'].dt.dayofyear
df['day_of_month'] = df['start_tm'].dt.day
df['day_of_week'] = df['start_tm'].dt.dayofweek

# Further preprocess
df['tndr_type'] = df['tndr_type'].replace('', 'Unknown').fillna('Unknown')
df['cshbk_amt'] = df['cshbk_amt'].fillna(0)
df['tm_disc'] = df['tm_disc'].fillna(0)

# Fill NaN values
df = df.fillna(0)
for column in df.select_dtypes(include=['object']).columns:
    if column not in FLAG_COLS:
        df[column] = df[column].replace('0', 'Unknown')

df.loc[df['register_i'].isin([61, 62, 63, 64]), 'cashier'] = 'Self_Checkout'
```

In [7]:
```
from sklearn.model_selection import train_test_split
from sklearn.preprocessing import MinMaxScaler

#Drop unnecessary columns
df.drop(columns=DROP_COLS, inplace=True)

# Get columns that are of 'object' dtype
columns_to_dummy = df.select_dtypes(include=['object']).columns

# Create dummy variables for the selected columns
df = pd.get_dummies(df, columns=columns_to_dummy).astype(int)

# Split data into training and validation sets (80% train, 20% validation)
train_data, val_data = train_test_split(df, test_size=0.2)

scaler = MinMaxScaler(feature_range=(-1, 1))
train_data_scaled = scaler.fit_transform(train_data)
val_data_scaled = scaler.transform(val_data)

train_data_scaled.shape, val_data_scaled.shape
```

Out[7]: ((928936, 735), (232234, 735))

Neural Networks

In [8]:
```
import torch
import torch.nn as nn
import torch.optim as optim
import torch.nn.functional as F
from torch.utils.data import DataLoader, TensorDataset
```

In [9]:
```python
# Hyperparameters
EPOCHS = 20
BATCH_SIZE = 128
LEARNING_RATE = 0.001
LOAD_MODEL = True
SAVE_MODEL = True

models = {}

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

In [10]:
```python
# Convert data to PyTorch tensors
train_dataset = TensorDataset(torch.tensor(train_data_scaled, dtype=torch.float32))
train_dataloader = DataLoader(train_dataset, batch_size=BATCH_SIZE, shuffle=True)
val_dataset = TensorDataset(torch.tensor(val_data_scaled, dtype=torch.float32))
val_dataloader = DataLoader(val_dataset, batch_size=BATCH_SIZE, shuffle=False)
```

Train/Val Functions

In [11]:
```python
from timeit import default_timer as timer
from tqdm.auto import tqdm
import matplotlib.pyplot as plt
```

In [12]:
```python
def train_step(model: torch.nn.Module,
               dataloader: torch.utils.data.DataLoader,
               loss_fn: torch.nn.Module,
               optimizer: torch.optim.Optimizer,
               device=device,
               sparse: bool = False):

    # Switch the model to train mode
    model.train()

    # Initialize variables to store total training loss
    train_loss = 0

    # Loop over batches from the DataLoader
    for batch, X in enumerate(dataloader):

        # Send batch of images to the computation device (CPU/GPU)
        X = X[0].to(device)

        # Perform a forward pass through the model to get the predictions
        outputs = model(X)

        # Calculate the loss between the predictions and actual values
        if sparse:
            X_pred = outputs
            loss = loss_fn(model, X_pred, X)
        else:
            X_pred = outputs
            loss = loss_fn(X_pred, X)

        # Add up the loss values
        train_loss += loss.item()

        # Reset the gradients from the previous iteration
        optimizer.zero_grad()

        # Perform backward propagation to calculate gradients
        loss.backward()

        # Perform a step of optimization
        optimizer.step()

    train_loss /= len(dataloader) # Calculate average training loss
    return train_loss # Return average training loss
```

In [13]:

```python
# Create eval_step() function
def val_step(model: torch.nn.Module,
             dataloader: torch.utils.data.DataLoader,
             loss_fn: torch.nn.Module,
             device=device,
             sparse: bool = False):

    # Switches the model to evaluation mode
    model.eval()

    # Initialize variables to store total test loss and accuracy
    val_loss = 0

    # Disable calculation of gradients for performance boost during inference
    with torch.inference_mode():

        # Loop over batches from the DataLoader
        for batch, X in enumerate(dataloader):

            # Send batch of images and labels to the computation device (CPU/GPU)
            X = X[0].to(device)

            # Perform a forward pass through the model to get the predictions
            outputs = model(X)

            # Calculate the loss between the predictions and actual values
            if sparse:
                X_pred = outputs
                loss = loss_fn(model, X_pred, X)
            else:
                X_pred = outputs
                loss = loss_fn(X_pred, X)
            # Add up the loss values
            val_loss += loss.item()

    val_loss /= len(dataloader) # Calculate average val loss
    return val_loss # Return average val loss
```

In [14]:

```python
# Create train() function
def train(model_name: str,
          model: torch.nn.Module,
          train_dataloader: torch.utils.data.DataLoader,
          val_dataloader: torch.utils.data.DataLoader,
          optimizer: torch.optim.Optimizer,
          loss_fn: torch.nn.Module,
          epochs: int = 5,
          device = device,
          sparse: bool = False,
          load_model: bool = True,
          save_model: bool = True,
          model_dir_path = model_dir_path):

    # Define the full model path including the file name
    model_path = os.path.join(model_dir_path, f"{model_name}.pth")

    # Initialize a dictionary to store training and validation losses and accuracies for each epoch
    results = {"train_loss": [],
               "val_loss": []}

    # Load the existing model and losses if required
    if load_model:
        loaded = load_model_fn(model, model_path, results)
        if loaded:
            return results


    # Establish the start time for training
    start_time = timer()

    # Loop over epochs
    for epoch in tqdm(range(epochs)):
        # Execute a training step and get training loss
        train_loss = train_step(model=model,
                                dataloader=train_dataloader,
                                loss_fn=loss_fn,
                                optimizer=optimizer,
                                device=device,
                                sparse=sparse)
        # Execute a validation step and get validation loss
        val_loss = val_step(model=model,
                            dataloader=val_dataloader,
                            loss_fn=loss_fn,
                            device=device,
                            sparse=sparse)
        # Print losses and accuracies for this epoch
        print(f"Epoch: {epoch} | Train loss: {train_loss:.4f} | Val loss: {val_loss:.4f}")

        # Append losses and accuracies to results dictionary
        results["train_loss"].append(train_loss)
        results["val_loss"].append(val_loss)

    # Establish the end time for training
    end_time = timer()
    train_time = end_time-start_time
    results['train_time'] = train_time

    if save_model:
        save_model_fn(model, model_path, results)

    return results
```

In [15]:

```python
def load_model_fn(model, model_path, results):
    if os.path.isfile(model_path):
        checkpoint = torch.load(model_path)
        model.load_state_dict(checkpoint['state_dict'])
        results['train_loss'] = checkpoint['train_loss']
        results['val_loss'] = checkpoint['val_loss']
        results['train_time'] = checkpoint['train_time']
        print(f"Model loaded from {model_path}")
        return True
    else:
        print(f"No existing model found at {model_path}. Training a new model.")
        return False
```

In [16]:
```python
def save_model_fn(model, model_path, results):
    save_dict = {
        'state_dict': model.state_dict(),
        'train_loss': results['train_loss'],
        'val_loss': results['val_loss'],
        'train_time': results['train_time']
    }
    torch.save(save_dict, model_path)
    print(f"Model saved at {model_path}")
```

In [17]:
```python
def plot_train_val_loss(results, model, image_dir_path=image_dir_path):
    plt.figure(figsize=(10,5))

    plt.plot(results['train_loss'], label='Training Loss')
    plt.plot(results['val_loss'], label='Validation Loss')

    plt.xlabel('Epoch')
    plt.ylabel('Loss')
    plt.title(f'Test and Validation Loss for {model}')
    plt.legend()

    save_plot(f"{model}_Train_Val_Loss", image_dir_path, plt)

    plt.show()
```

Model 1

Regular Autoencoder

In [18]:
```python
# Define the autoencoder model
class Autoencoder(torch.nn.Module):
    def __init__(self, input_dim):
        super(Autoencoder, self).__init__()
        self.encoder = nn.Sequential(
            nn.Linear(input_dim, 256),
            nn.ReLU(),

            nn.Linear(256, 128),
            nn.ReLU(),

            nn.Linear(128, 64),
            nn.ReLU(),

            nn.Linear(64, 32),
            nn.ReLU(),

            nn.Linear(32, 16),
            nn.ReLU(),
        )
        self.decoder = nn.Sequential(
            nn.Linear(16, 32),
            nn.ReLU(),

            nn.Linear(32, 64),
            nn.ReLU(),

            nn.Linear(64, 128),
            nn.ReLU(),

            nn.Linear(128, 256),
            nn.ReLU(),

            nn.Linear(256, input_dim),
            nn.Tanh(),
        )

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

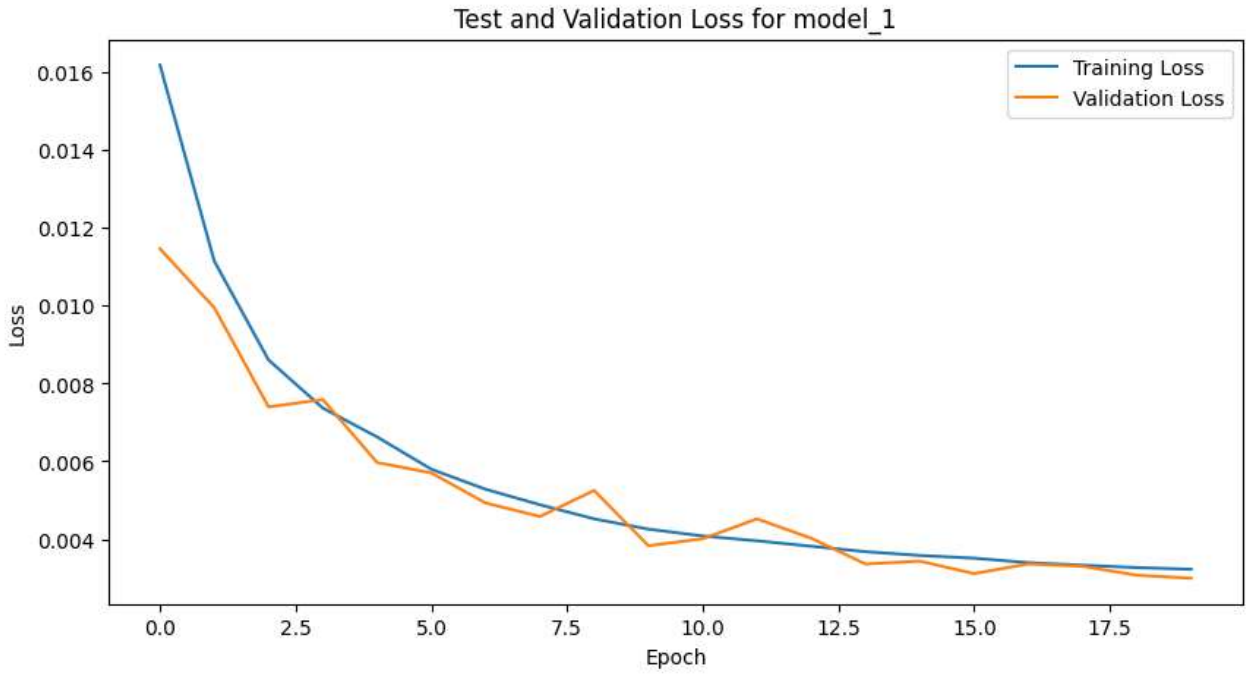
In [19]:
```
# Initialize the model, loss function and optimizer
model_1 = Autoencoder(input_dim=train_data_scaled.shape[1])
loss_fn_1 = nn.MSELoss()
optimizer_1 = optim.Adam(model_1.parameters(), lr=LEARNING_RATE)

# Move model to appropriate device
model_1.to(device)
models["model_1"]=model_1
```

In [20]:
```
model_1_results = train(model_name = list(models.keys())[0],
                        model=model_1,
                        train_dataloader=train_dataloader,
                        val_dataloader=val_dataloader,
                        optimizer=optimizer_1,
                        loss_fn=loss_fn_1,
                        epochs=EPOCHS,
                        device=device,
                        load_model=LOAD_MODEL,
                        save_model=SAVE_MODEL)
```

```
Model loaded from models\All_Purchases\model_1.pth
```

In [21]:
```
plot_train_val_loss(model_1_results, list(models.keys())[0])
```

```
Image has been saved at Images\All_Purchases\model_1_Train_Val_Loss
```



Model 2

Deeper autoencoder with dropout and normalization

In [22]:

```python
# Define the autoencoder model
import torch.nn as nn

class DeepAutoencoder(torch.nn.Module):
    def __init__(self, input_dim):
        super(DeepAutoencoder, self).__init__()

        # Encoder
        self.encoder = nn.Sequential(
            nn.Linear(input_dim, 512),
            nn.ReLU(),
            nn.BatchNorm1d(512),
            nn.Dropout(0.5),

            nn.Linear(512, 256),
            nn.ReLU(),
            nn.BatchNorm1d(256),
            nn.Dropout(0.5),

            nn.Linear(256, 128),
            nn.ReLU(),
            nn.BatchNorm1d(128),
            nn.Dropout(0.5),

            nn.Linear(128, 64),
            nn.ReLU(),
            nn.BatchNorm1d(64),

            nn.Linear(64, 32),
            nn.ReLU(),
            nn.BatchNorm1d(32),

            nn.Linear(32, 16),
            nn.ReLU(),
            nn.BatchNorm1d(16)
        )

        # Decoder
        self.decoder = nn.Sequential(
            nn.Linear(16, 32),
            nn.ReLU(),
            nn.BatchNorm1d(32),

            nn.Linear(32, 64),
            nn.ReLU(),
            nn.BatchNorm1d(64),

            nn.Linear(64, 128),
            nn.ReLU(),
            nn.BatchNorm1d(128),

            nn.Linear(128, 256),
            nn.ReLU(),
            nn.BatchNorm1d(256),

            nn.Linear(256, input_dim),
            nn.Tanh()
        )

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

In [23]:

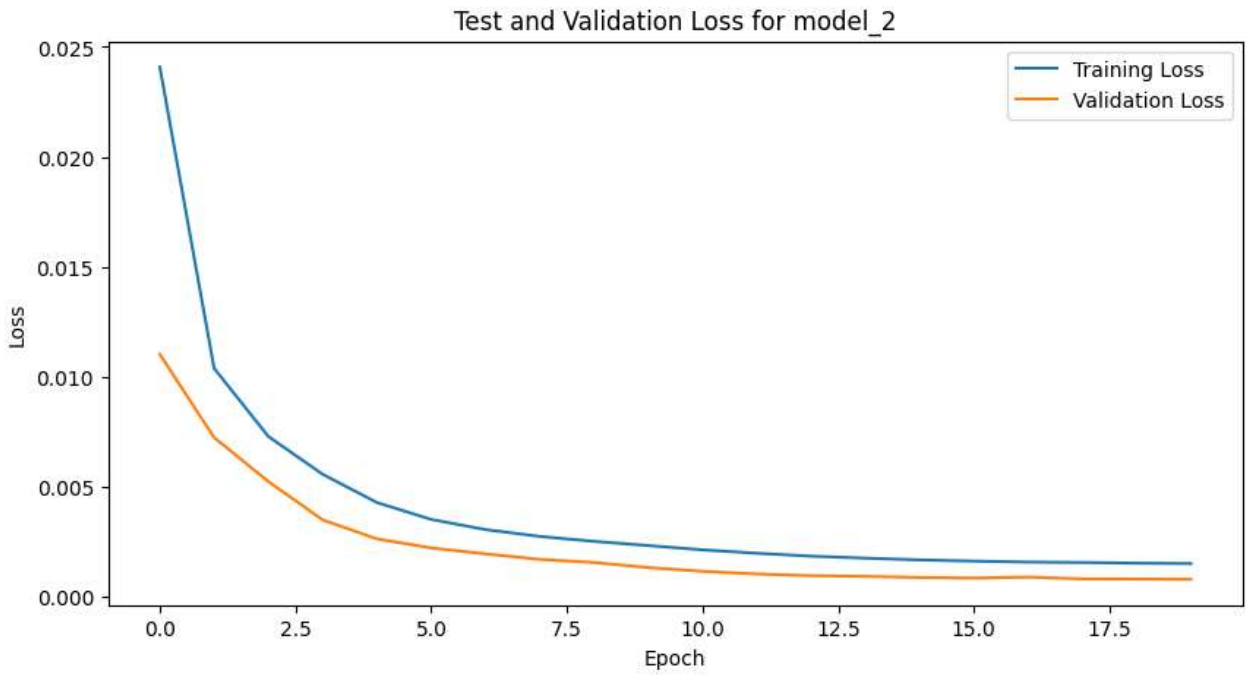
```python
# Initialize the model, loss function and optimizer
model_2 = DeepAutoencoder(input_dim=train_data_scaled.shape[1])
loss_fn_2 = nn.MSELoss()
optimizer_2 = optim.Adam(model_2.parameters(), lr=LEARNING_RATE)

# Move model to appropriate device
model_2.to(device)
models["model_2"]=model_2
```

In [24]:
```
model_2_results = train(model_name = list(models.keys())[1],
                        model=model_2,
                        train_dataloader=train_dataloader,
                        val_dataloader=val_dataloader,
                        optimizer=optimizer_2,
                        loss_fn=loss_fn_2,
                        epochs=EPOCHS,
                        device=device,
                        load_model=LOAD_MODEL,
                        save_model=SAVE_MODEL)
```

```
Model loaded from models\All_Purchases\model_2.pth
```

In [25]:
```
plot_train_val_loss(model_2_results, list(models.keys())[1])
```

```
Image has been saved at Images\All_Purchases\model_2_Train_Val_Loss
```



Model 3

Denoising Autoencoder

In [26]:

```python
class DenoisingAutoencoder(nn.Module):
    def __init__(self, input_dim, noise_factor=0.5):
        super(DenoisingAutoencoder, self).__init__()
        self.noise_factor = noise_factor
        # Encoder
        self.encoder = nn.Sequential(
            nn.Linear(input_dim, 512),
            nn.ReLU(),
            nn.BatchNorm1d(512),
            nn.Dropout(0.5),

            nn.Linear(512, 256),
            nn.ReLU(),
            nn.BatchNorm1d(256),
            nn.Dropout(0.5),

            nn.Linear(256, 128),
            nn.ReLU(),
            nn.BatchNorm1d(128),
            nn.Dropout(0.5),

            nn.Linear(128, 64),
            nn.ReLU(),
            nn.BatchNorm1d(64),

            nn.Linear(64, 32),
            nn.ReLU(),
            nn.BatchNorm1d(32),

            nn.Linear(32, 16),
            nn.ReLU(),
            nn.BatchNorm1d(16)
        )

        # Decoder
        self.decoder = nn.Sequential(
            nn.Linear(16, 32),
            nn.ReLU(),
            nn.BatchNorm1d(32),

            nn.Linear(32, 64),
            nn.ReLU(),
            nn.BatchNorm1d(64),

            nn.Linear(64, 128),
            nn.ReLU(),
            nn.BatchNorm1d(128),

            nn.Linear(128, 256),
            nn.ReLU(),
            nn.BatchNorm1d(256),

            nn.Linear(256, input_dim),
            nn.Tanh()
        )

    def forward(self, x):
        x_noisy = x + self.noise_factor * torch.randn_like(x)  # Add noise to the input
        x_noisy = torch.clamp(x_noisy, 0., 1.)  # Ensure the noisy input values are between 0 and 1.
        x_encoded = self.encoder(x_noisy)  # Encode the noisy input
        x_decoded = self.decoder(x_encoded)  # Decode the encoded representation
        return x_decoded
```

In [27]:

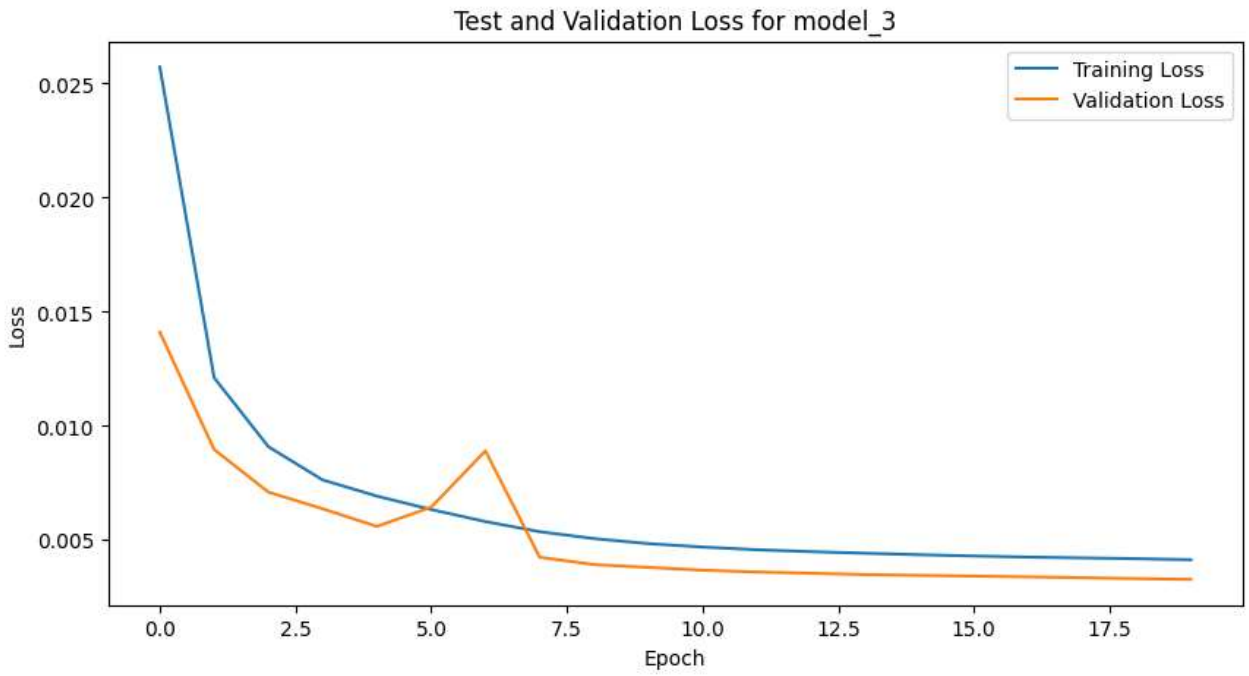
```python
# Initialize the model, loss function and optimizer
model_3 = DenoisingAutoencoder(input_dim=train_data_scaled.shape[1])
loss_fn_3 = nn.MSELoss()
optimizer_3 = optim.Adam(model_3.parameters(), lr=LEARNING_RATE)

# Move model to appropriate device
model_3.to(device)
models["model_3"]=model_3
```

In [28]:
```
model_3_results = train(model_name = list(models.keys())[2],
                        model=model_3,
                        train_dataloader=train_dataloader,
                        val_dataloader=val_dataloader,
                        optimizer=optimizer_3,
                        loss_fn=loss_fn_3,
                        epochs=EPOCHS,
                        device=device,
                        load_model=LOAD_MODEL,
                        save_model=SAVE_MODEL)
```

```
Model loaded from models\All_Purchases\model_3.pth
```

In [29]:
```
plot_train_val_loss(model_3_results, list(models.keys())[2])
```

```
Image has been saved at Images\All_Purchases\model_3_Train_Val_Loss
```



Model 4

Sparse Autoencoder

In [30]:

```python
class SparseAutoencoder(nn.Module):
    def __init__(self, input_dim):
        super(SparseAutoencoder, self).__init__()
        # Encoder
        self.encoder = nn.Sequential(
            nn.Linear(input_dim, 512),
            nn.ReLU(),
            nn.BatchNorm1d(512),
            nn.Dropout(0.5),

            nn.Linear(512, 256),
            nn.ReLU(),
            nn.BatchNorm1d(256),
            nn.Dropout(0.5),

            nn.Linear(256, 128),
            nn.ReLU(),
            nn.BatchNorm1d(128),
            nn.Dropout(0.5),

            nn.Linear(128, 64),
            nn.ReLU(),
            nn.BatchNorm1d(64),

            nn.Linear(64, 32),
            nn.ReLU(),
            nn.BatchNorm1d(32),

            nn.Linear(32, 16),
            nn.ReLU(),
            nn.BatchNorm1d(16)
        )

        # Decoder
        self.decoder = nn.Sequential(
            nn.Linear(16, 32),
            nn.ReLU(),
            nn.BatchNorm1d(32),

            nn.Linear(32, 64),
            nn.ReLU(),
            nn.BatchNorm1d(64),

            nn.Linear(64, 128),
            nn.ReLU(),
            nn.BatchNorm1d(128),

            nn.Linear(128, 256),
            nn.ReLU(),
            nn.BatchNorm1d(256),

            nn.Linear(256, input_dim),
            nn.Tanh()
        )

    def forward(self, x):
        x = self.encoder(x)
        self.mean_activation = torch.mean(x, dim=0)  # Compute the mean activation
        x = self.decoder(x)
        return x
```

In [31]:

```python
def sparse_loss_fn(model, X, X_pred, beta=1e-3, rho=0.05, epsilon=1e-7):
    # Reconstruction loss
    mse_loss = nn.MSELoss()(X_pred, X)

    # Ensure mean_activation is not exactly 0 or 1
    mean_activation = torch.clamp(model.mean_activation, min=epsilon, max=1-epsilon)

    # Sparsity loss
    sparsity_loss = torch.abs(torch.sum(rho * torch.log(rho / mean_activation) + (1 - rho) * torch.log((1 - rho) / (1 - mea

    # Total loss
    total_loss = mse_loss + beta * sparsity_loss

    return total_loss
```

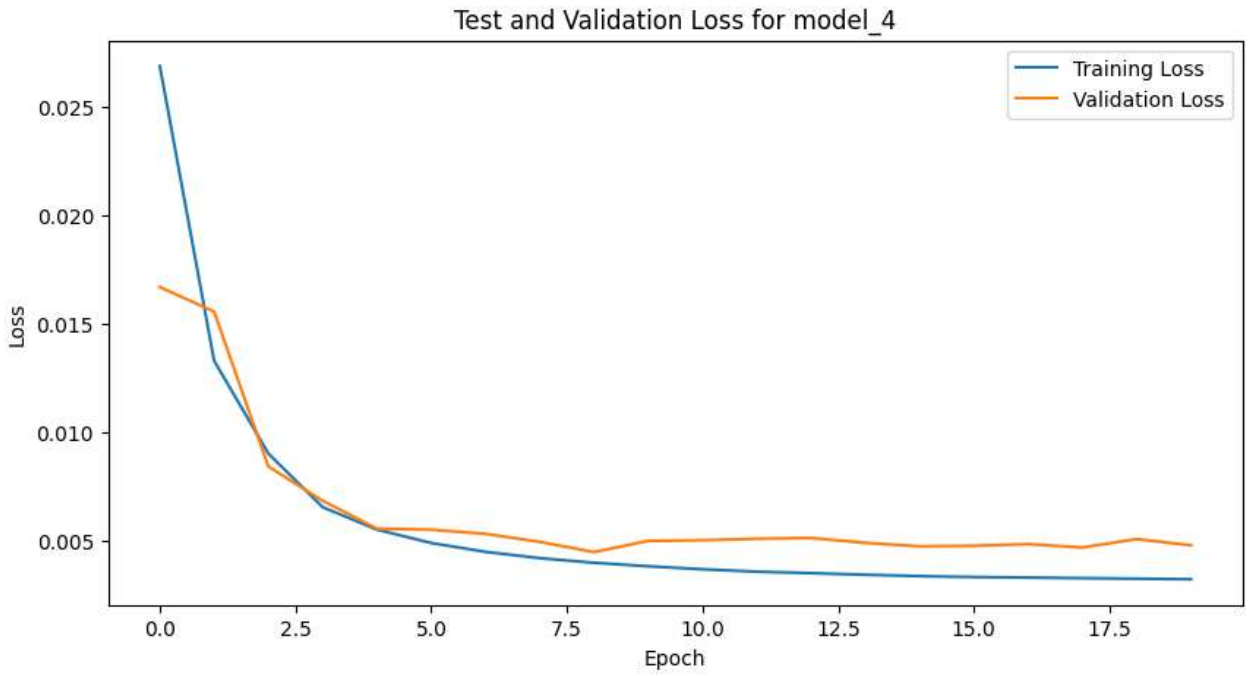
In [32]:
```
# Initialize the model, loss function and optimizer
model_4 = SparseAutoencoder(input_dim=train_data_scaled.shape[1])
loss_fn_4 = sparse_loss_fn
optimizer_4 = optim.Adam(model_4.parameters(), lr=LEARNING_RATE)

# Move model to appropriate device
model_4.to(device)
models["model_4"]=model_4
```

In [33]:
```
model_4_results = train(model_name = list(models.keys())[3],
                        model=model_4,
                        train_dataloader=train_dataloader,
                        val_dataloader=val_dataloader,
                        optimizer=optimizer_4,
                        loss_fn=loss_fn_4,
                        epochs=EPOCHS,
                        device=device,
                        sparse=True,
                        load_model=LOAD_MODEL,
                        save_model=SAVE_MODEL)
```

```
Model loaded from models\All_Purchases\model_4.pth
```

In [34]:
```
plot_train_val_loss(model_4_results, list(models.keys())[3])
```

```
Image has been saved at Images\All_Purchases\model_4_Train_Val_Loss
```



Comparison Graphs

In [35]:

```python
# Create a dictionary of model results
model_dict = {
    'model_1': model_1_results,
    'model_2': model_2_results,
    'model_3': model_3_results,
    'model_4': model_4_results
}

final_results = {
    model_name: {
        key: value[-1] if isinstance(value, list) and len(value) > 1 else value
        for key, value in model.items()
    }
    for model_name, model in model_dict.items()
}

# Create DataFrame with correct orientation and add training time
results = pd.DataFrame(final_results).T

results
```

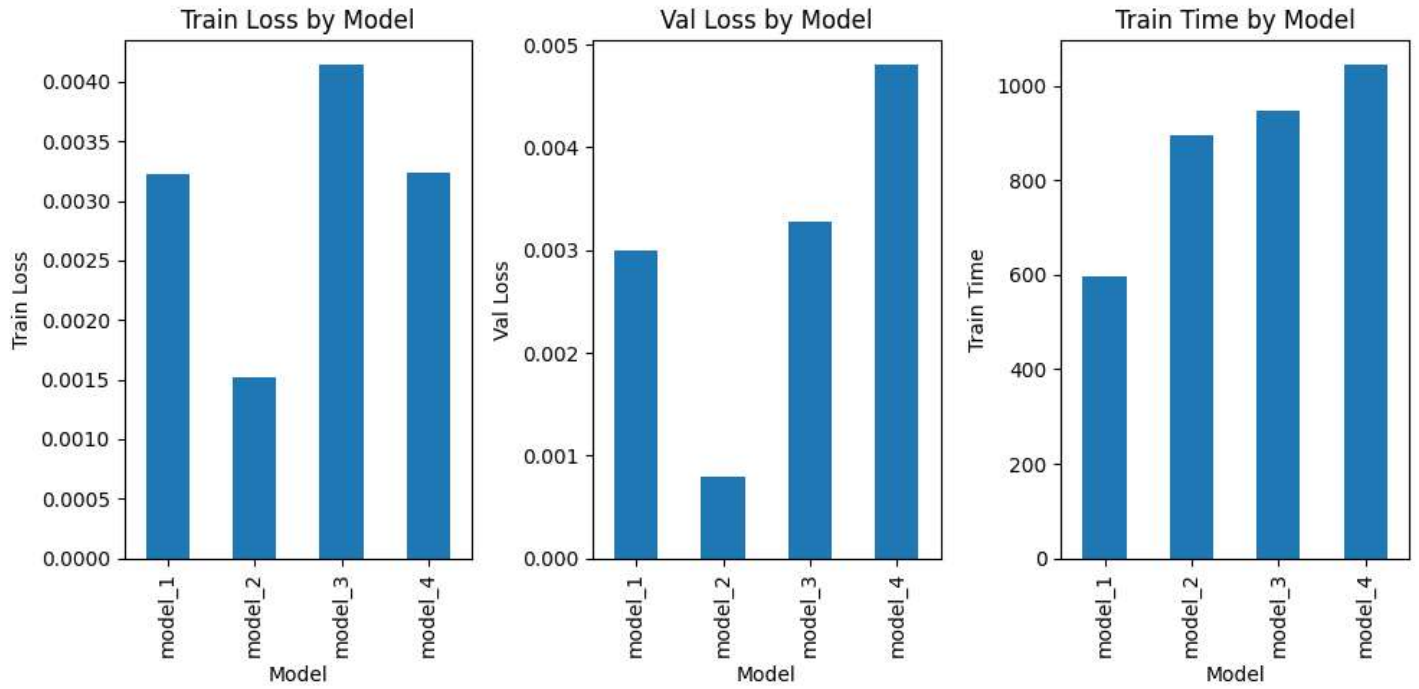
Out[35]:

	train_loss	val_loss	train_time
model_1	0.003226	0.002995	597.201953
model_2	0.001518	0.000798	896.574678
model_3	0.004138	0.003279	946.267649
model_4	0.003234	0.004800	1043.932900

In [36]:

```
plt.figure(figsize=(10,5))

plt.subplot(1, 3, 1)
results['train_loss'].plot(kind='bar')
plt.xlabel('Model')
plt.ylabel('Train Loss')
plt.title('Train Loss by Model')

plt.subplot(1, 3, 2)
results['val_loss'].plot(kind='bar')
plt.xlabel('Model')
plt.ylabel('Val Loss')
plt.title('Val Loss by Model')

plt.subplot(1, 3, 3)
results['train_time'].plot(kind='bar')
plt.xlabel('Model')
plt.ylabel('Train Time')
plt.title('Train Time by Model')

plt.tight_layout()  # Adjusts spacing between subplots for better layout
file_name = "TrainLoss_ValLoss_TrainTime"

save_plot("TrainLoss_ValLoss_TrainTime_Bar", image_dir_path, plt)

plt.show()
```

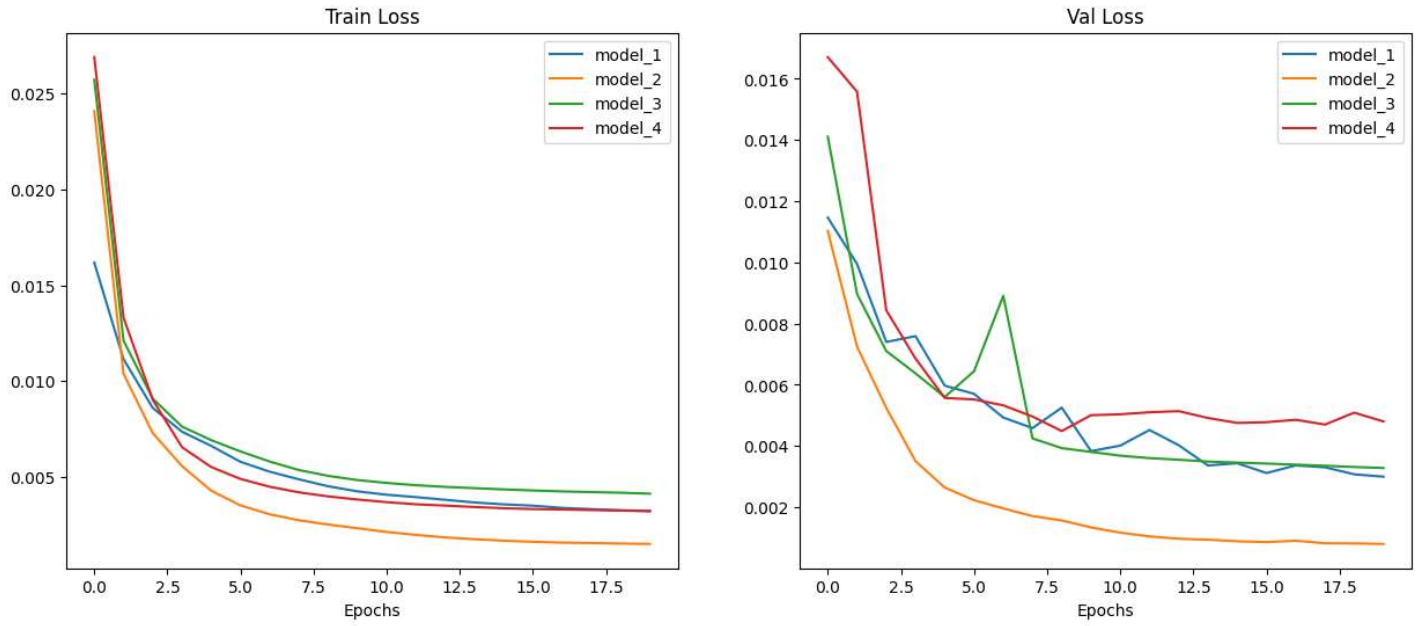
```
Image has been saved at Images\All_Purchases\TrainLoss_ValLoss_TrainTime_Bar
```



In [37]:

```
# Setup a plot
plt.figure(figsize=(15,6))

# Get number of epochs
epochs = range(len(model_1_results["train_loss"]))

# Plot train loss
plt.subplot(1, 2, 1)
for i in range(len(model_dict)):
    plt.plot(epochs, model_dict[list(model_dict)[i]]['train_loss'], label=list(model_dict)[i])
plt.title("Train Loss")
plt.xlabel("Epochs")
plt.legend()

# Plot val loss
plt.subplot(1, 2, 2)
for i in range(len(model_dict)):
    plt.plot(epochs, model_dict[list(model_dict)[i]]['val_loss'], label=list(model_dict)[i])
plt.title("Val Loss")
plt.xlabel("Epochs")
plt.legend()

save_plot("TrainLoss_ValLoss_Line", image_dir_path, plt)

plt.show()
```

```
Image has been saved at Images\All_Purchases\TrainLoss_ValLoss_Line
```



Graphing in Latent Space

In [38]:

```python
import numpy as np
import matplotlib.pyplot as plt
from sklearn.decomposition import PCA
from sklearn.cluster import KMeans
from tqdm import tqdm
import torch
from torch import linalg as LA

def apply_pca_optimized(data, n_components=None, visualize=True, labels=None, image_dir_path=image_dir_path):
    """
    Apply Principal Component Analysis (PCA) on the given data and optionally visualize the results.
    The data will be reduced to 2 dimensions for visualization.

    :param data: Input data to apply PCA on.
    :param n_components: Number of principal components to consider for transformation. If None, use all components.
    :param visualize: Whether to visualize the results. Defaults to True.
    :return: Transformed data after applying PCA.
    """
    # Apply PCA using sklearn
    pca = PCA(n_components=n_components)
    transformed_data = pca.fit_transform(data)

    # Visualize the results if required
    if visualize:
        visualize_pca(transformed_data, labels, image_dir_path)

    # Print the total explained variance
    print("Total Explained Variance ({} components): {:.2%}".format(n_components if n_components else data.shape[1], np.sum

    return transformed_data

def visualize_pca(transformed_data, labels=None, image_dir_path=image_dir_path):
    """Visualize the PCA results in 2D space."""
    # Apply PCA for 2D visualization
    pca_2d = PCA(n_components=2)
    transformed_data_2d = pca_2d.fit_transform(transformed_data)

    plt.figure(figsize=(10,10))
    plt.scatter(transformed_data_2d[:, 0], transformed_data_2d[:, 1], c=labels, s=1, cmap='viridis')
    plt.xlabel("Principal Component 1")
    plt.ylabel("Principal Component 2")
    plt.title("2D PCA Projection")

    if labels is not None:
        save_plot("PCA_Visualization_Labels", image_dir_path, plt)
    else:
        save_plot("PCA_Visualization", image_dir_path, plt)

    plt.show()

def plot_cumulative_variance(data, max_components=15, image_dir_path=image_dir_path):
    """
    Plot cumulative explained variance against the number of components.
    """
    # Convert data to PyTorch tensor and move to the device
    data_tensor = torch.tensor(data, dtype=torch.float32).to(device)

    # Center the data
    mean_centered_data = data_tensor - data_tensor.mean(dim=0)

    # Compute the covariance matrix
    covariance_matrix = torch.mm(mean_centered_data.T, mean_centered_data) / (data_tensor.size(0) - 1)

    # Compute eigenvalues
    eigenvalues, _ = LA.eig(covariance_matrix)
    eigenvalues = torch.real(eigenvalues)

    # Sort the eigenvalues in descending order
    sorted_eigenvalues, _ = torch.sort(eigenvalues, descending=True)

    # Compute the cumulative explained variance
    cumulative_explained_variances = torch.cumsum(sorted_eigenvalues, dim=0) / torch.sum(sorted_eigenvalues)

    # Plotting
    plt.figure(figsize=(10,6))
    plt.plot(range(1, max_components+1), cumulative_explained_variances[:max_components].cpu().numpy(), marker='o')
    plt.title("Cumulative Explained Variance vs. Number of Components")
    plt.xlabel("Number of Components")
    plt.ylabel("Cumulative Explained Variance")
    plt.ylim(0, 1)
    plt.grid(True)

    save_plot("Cumulative_Variance", image_dir_path, plt)

```

```
    plt.show()

def plot_clusters(data, max_clusters=10, image_dir_path=image_dir_path):
    """
    Display a line graph with points to visualize the sum of squared distances (SSD) for different cluster numbers.
    """
    # Compute the SSD for the range of clusters
    ssd = [KMeans(n_clusters=k, n_init=10).fit(data).inertia_ for k in range(1, max_clusters+1)]

    # Visualization
    k_values = range(1, max_clusters+1)
    plt.figure(figsize=(6, 6))
    plt.plot(k_values, ssd, '-')
    plt.scatter(k_values, ssd, color='b')
    plt.title('Sum of Squared Distances vs Number of Clusters')
    plt.xlabel('Number of clusters')
    plt.ylabel('Sum of squared distances')
    plt.grid(True)

    save_plot("Cluster_Plot", image_dir_path, plt)

    plt.show()
```

Finding top 3 anomalous columns

In [39]:

```
# Combine training and validation data
df_scaled = scaler.fit_transform(df)

# Convert data to PyTorch tensors
dataset = TensorDataset(torch.tensor(df_scaled, dtype=torch.float32))
dataloader = DataLoader(dataset, batch_size=BATCH_SIZE, shuffle=False)
```

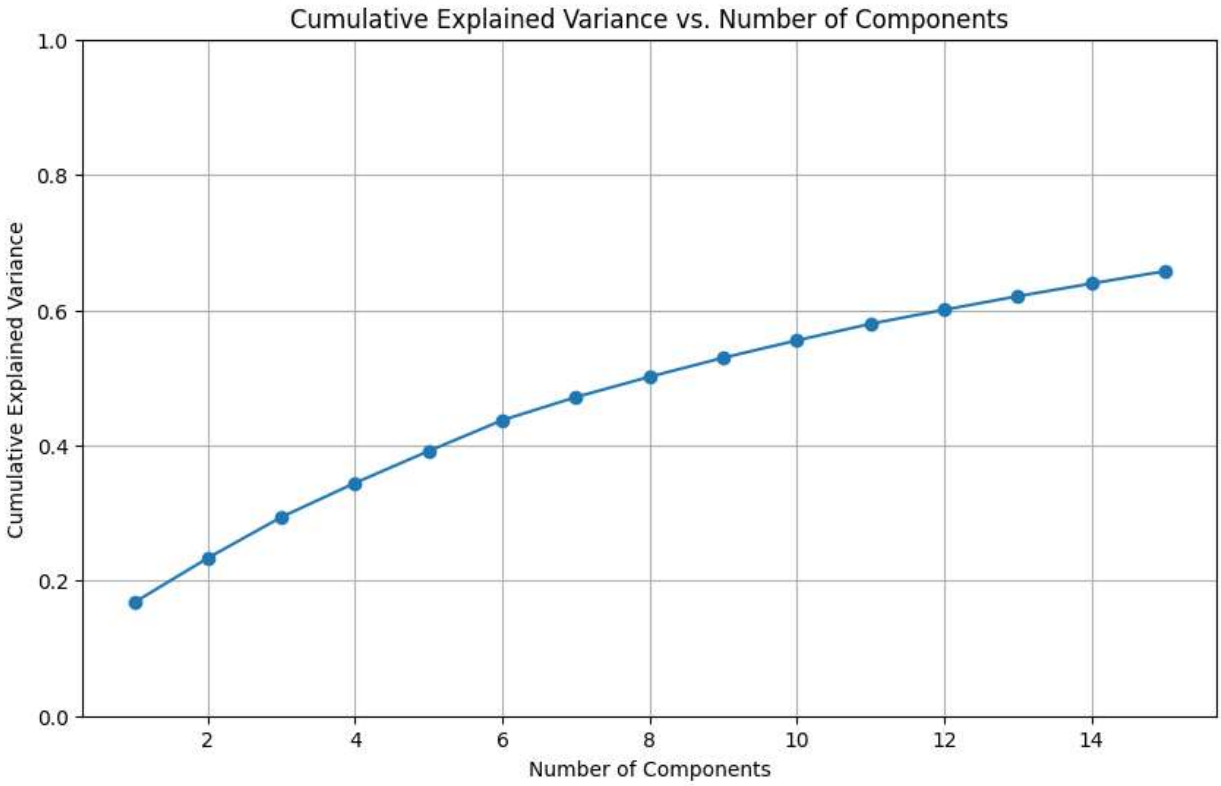
In [40]:

```python
import torch

def calculate_reconstruction_and_top_3_values(model_name, model, dataloader, df_scaled, device):
    reconstructed_batches = []
    model.eval()
    with torch.inference_mode():
        for batch_data in tqdm(dataloader, desc=f'Processing {model_name}'):
            inputs = batch_data[0].to(device)
            reconstructed_batch = model(inputs)
            reconstructed_batches.append(reconstructed_batch)

    reconstructed = torch.cat(reconstructed_batches, dim=0).to(device)

    # Reconstruction error calculation
    reconstruction_error = ((reconstructed - torch.tensor(df_scaled, dtype=torch.float32).to(device)) ** 2).mean(dim=1).cpu

    # Top 3 values calculation
    difference_percentage = 100 * (reconstructed - torch.tensor(df_scaled, dtype=torch.float32).to(device)) / (torch.tensor
    difference_df = pd.DataFrame(difference_percentage.cpu().numpy())

    # Ensure that difference_df is a tensor
    difference_tensor = torch.tensor(difference_df.values).to(device)

    # Compute the absolute value
    abs_difference_tensor = torch.abs(difference_tensor)

    # Determine the top 3 maximum absolute differences and their indices for each row
    top_3_max_diff_values, indices = torch.topk(abs_difference_tensor, 3, dim=1)

    # Convert the indices to column names
    top_3_column_names_from_df = [[df.columns[i] for i in row] for row in indices.cpu().numpy()]

    # Separate the values for each top 3 column
    top_3_values = top_3_max_diff_values.cpu().numpy()

    # Create a new DataFrame to store the top 3 max column names and values
    top_3_max_diff_df = pd.DataFrame({
        'Top_1_Column': [row[0] for row in top_3_column_names_from_df],
        'Top_1_Value': top_3_values[:, 0],
        'Top_2_Column': [row[1] for row in top_3_column_names_from_df],
        'Top_2_Value': top_3_values[:, 1],
        'Top_3_Column': [row[2] for row in top_3_column_names_from_df],
        'Top_3_Value': top_3_values[:, 2],
    })

    return reconstruction_error, top_3_max_diff_df
```

PCA Analysis

In [41]:
```
1 plot_cumulative_variance(df_scaled)
```

```
Image has been saved at Images\All_Purchases\Cumulative_Variance
```



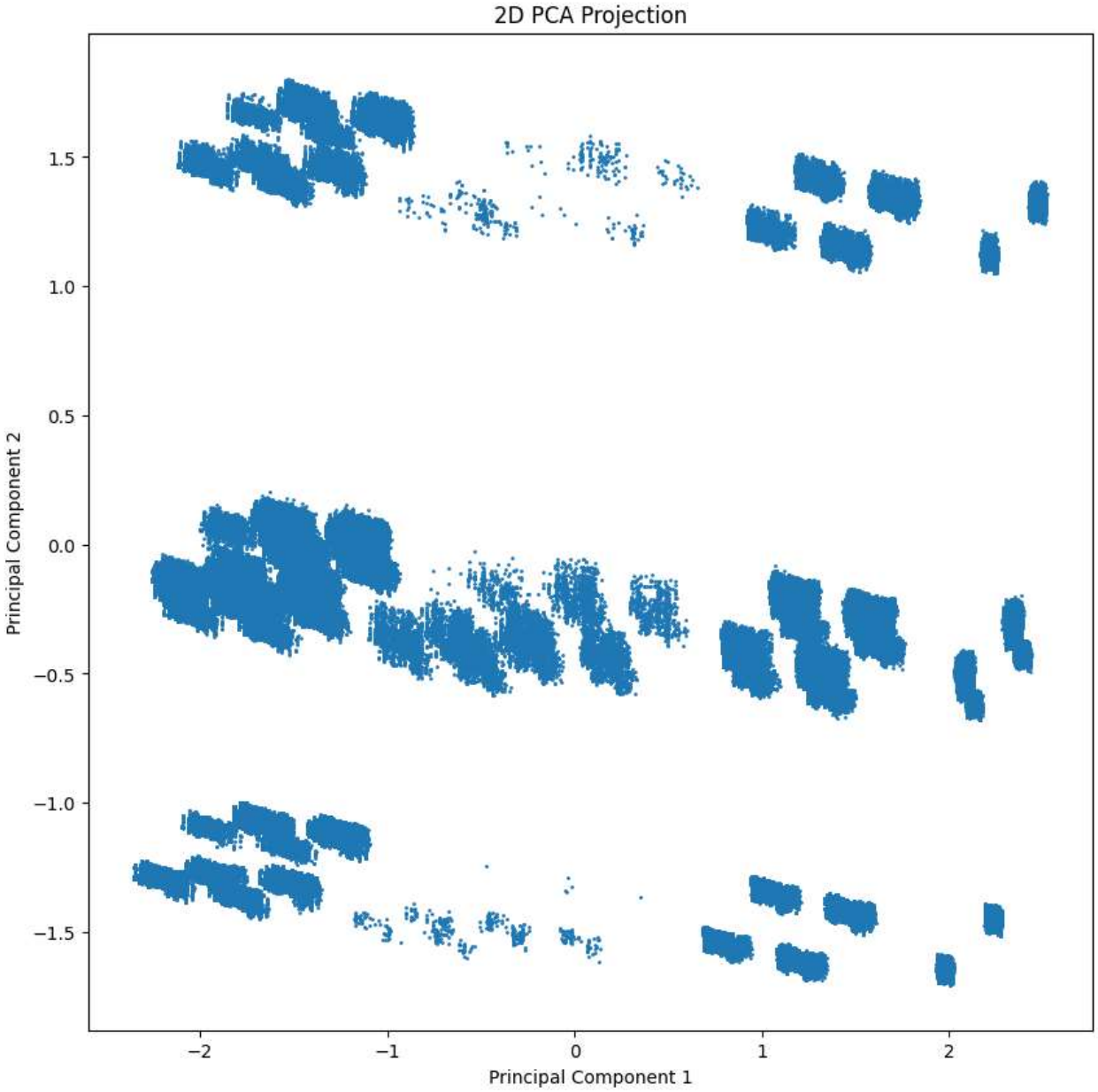
In [42]:
```
1 dim_input = int(input("Please enter the number of dimensions: "))
```

```
Please enter the number of dimensions: 9
```

In [43]:

```
# PCA Analysis
import warnings

with warnings.catch_warnings():
    warnings.simplefilter("ignore")
    transformed_data = apply_pca_optimized(df_scaled, n_components=dim_input)
```

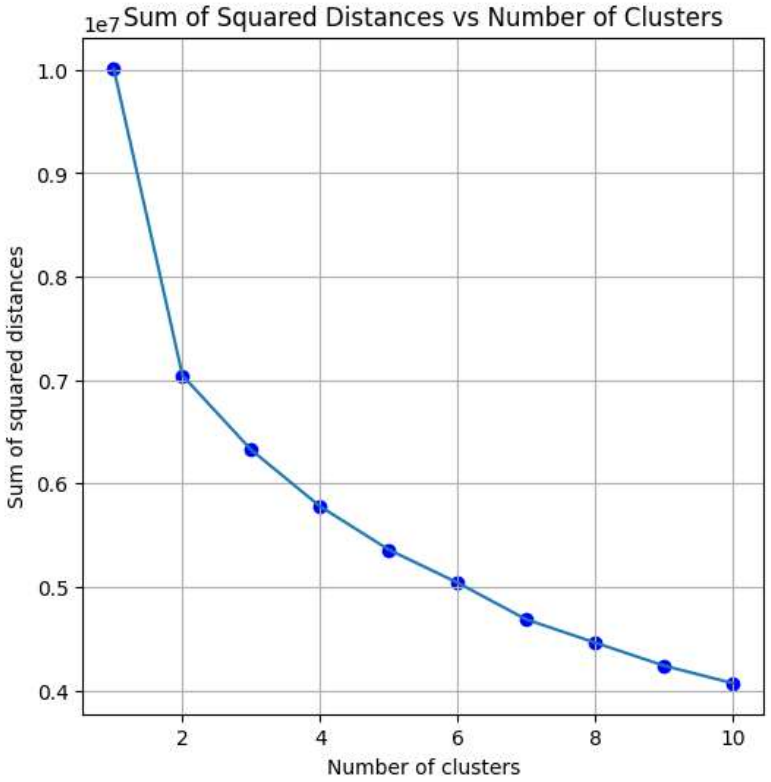
```
Image has been saved at Images\All_Purchases\PCA_Visualization
```




```
Total Explained Variance (9 components): 52.95%
```

In [44]:
```
# Visualize Cluster SSD
plot_clusters(transformed_data)
```

```
Image has been saved at Images\All_Purchases\Cluster_Plot
```



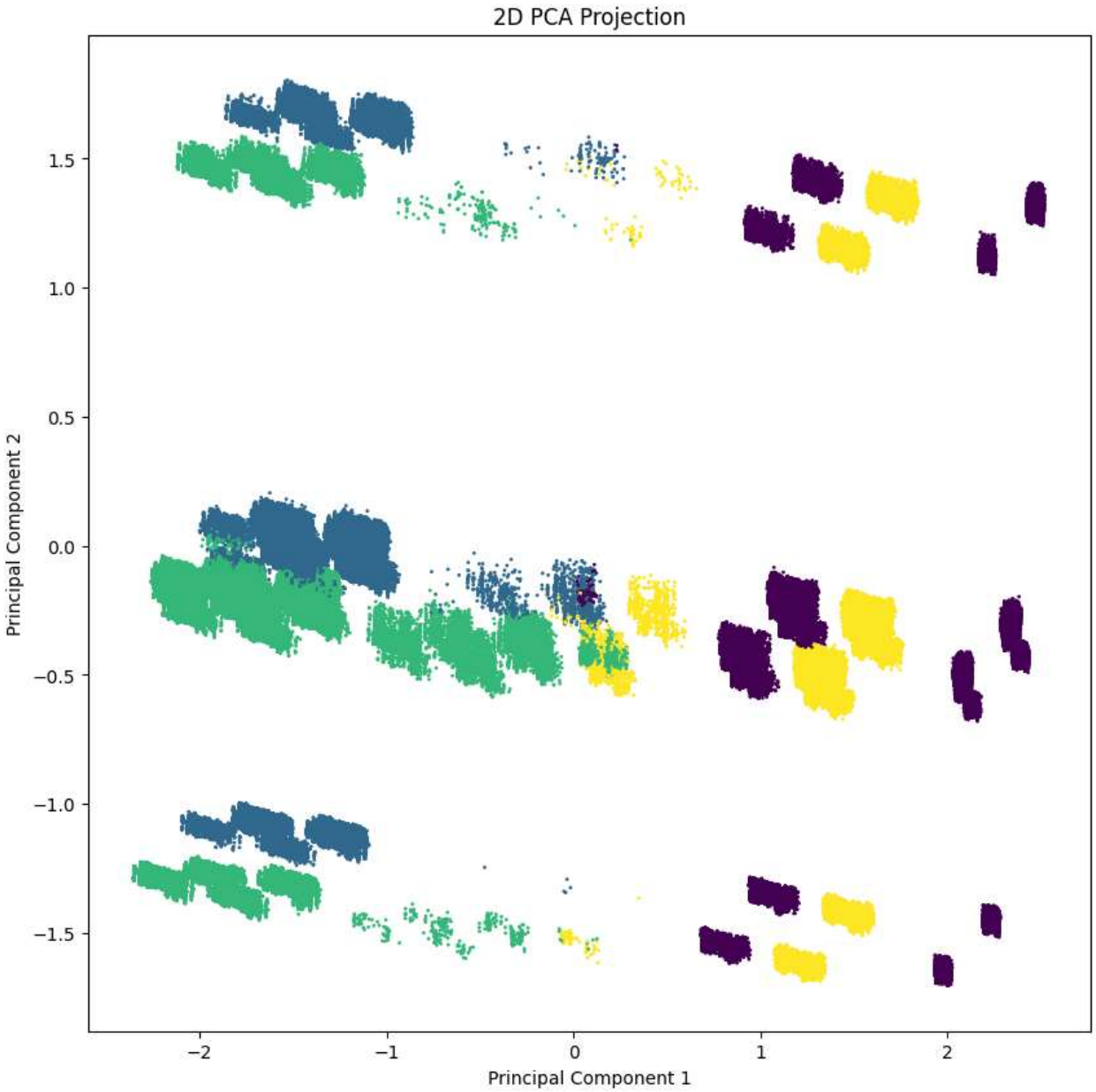
In [45]:
```
cluster_input = int(input("Please enter the number of clusters: "))
```

```
Please enter the number of clusters: 4
```

In [46]:
```
kmeans = KMeans(n_clusters=cluster_input, n_init=10)
kmeans.fit(transformed_data)
labels = kmeans.labels_
df_labels = pd.DataFrame(labels, columns=['PCA_Labels'])
```

In [47]:
```
1 visualize_pca(transformed_data, labels=labels)
```

```
Image has been saved at Images\All_Purchases\PCA_Visualization_Labels
```

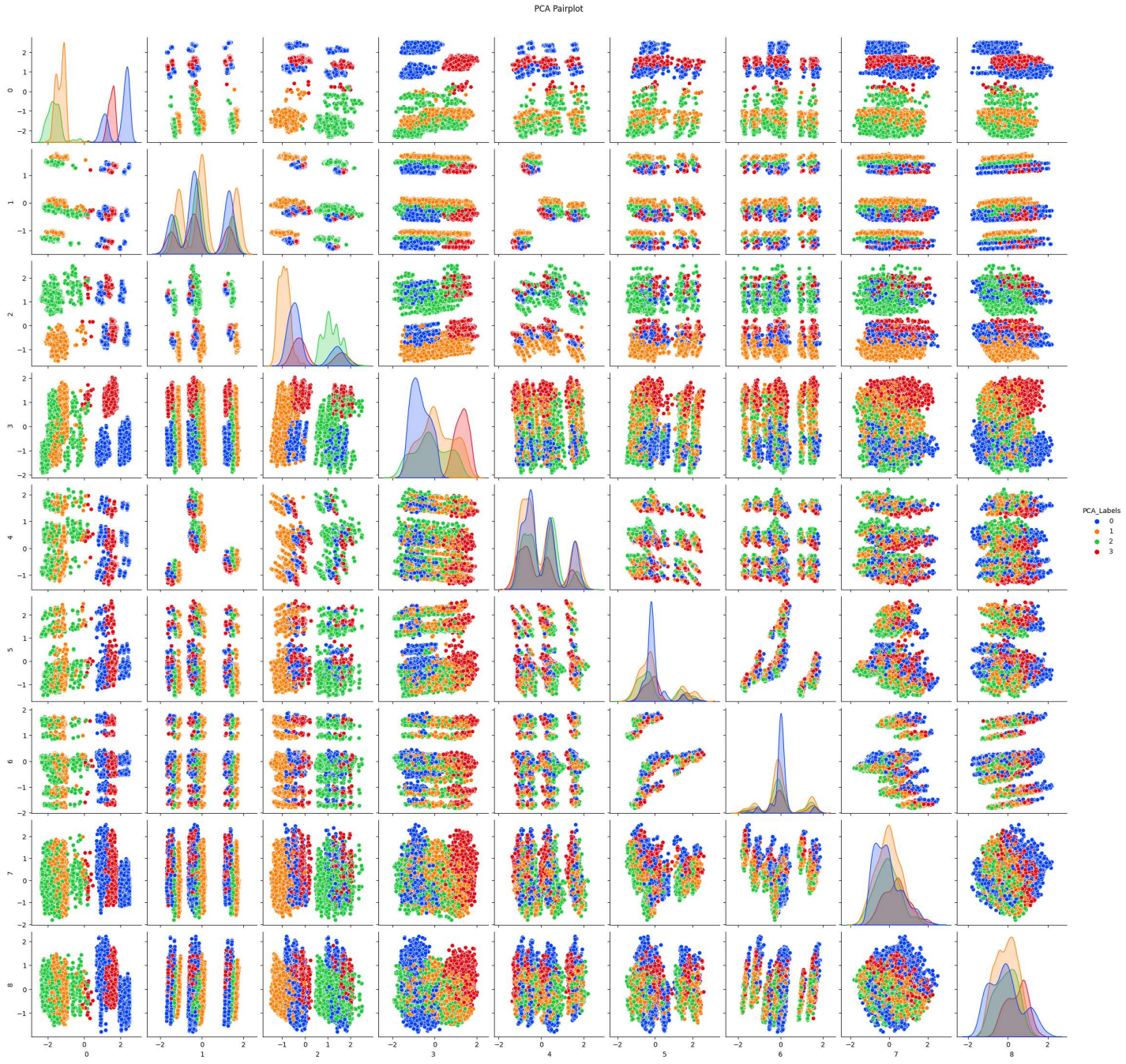


In [48]:
```
1 df_transformed_data = pd.DataFrame(transformed_data)
2 df_transformed_data['PCA_Labels'] = labels
3 sampled_data = df_transformed_data.sample(n=10000)
```

In [49]:

```
import seaborn as sns

# Create the pairplot
with warnings.catch_warnings():
    warnings.simplefilter("ignore")
    plot = sns.pairplot(sampled_data, hue='PCA_Labels', palette="bright")

    # Adjusting space at the top for the title
    plt.subplots_adjust(top=0.95)
    plt.suptitle("PCA Pairplot")

    # Call the save_plot function to save the image, with the correct file extension
    save_plot("PCA_Pairplot", image_dir_path, plot.fig)
```

```
Image has been saved at Images\All_Purchases\PCA_Pairplot
```



Finding anomalies

In [50]:

```python
from tqdm.notebook import tqdm
import os
import numpy as np
import pandas as pd
from datetime import datetime, timedelta

def detect_anomalies(reconstruction_error, threshold):
    anomaly_threshold = np.percentile(reconstruction_error, threshold)
    return reconstruction_error > anomaly_threshold

def create_dataframe(reconstruction_error, df_orig, df_top_3, df_labels):
    scores_df = pd.DataFrame(reconstruction_error, columns=['anomaly_score'])
    df_score = pd.concat([scores_df, df_orig, df_top_3, df_labels], axis=1)
    return df_score

def save_anomalies(all_anomalies, model_name, filename, result_dir_path=None):
    if result_dir_path is None:
        raise ValueError("result_dir_path must be provided.")
    dir_path = os.path.join(result_dir_path, model_name)
    os.makedirs(dir_path, exist_ok=True)
    all_anomalies.to_csv(os.path.join(dir_path, filename), index=False)

def filter_recent_anomalies(all_anomalies):
    cutoff_date = datetime.now() - timedelta(days=30)
    all_anomalies['sls_d'] = pd.to_datetime(all_anomalies['sls_d'])
    df_filtered = all_anomalies[all_anomalies['sls_d'] >= cutoff_date]
    return df_filtered.sort_values(by=['anomaly_score', 'sls_d', 'start_tm'], ascending=[False, False, True])

def detect_and_save_anomalies(model_name, model, dataloader, df_top_3, labels, df_orig, threshold=99.9, result_dir_path=Non
    if reconstruction_error is None:
        raise ValueError("reconstruction_error must be provided.")
    if result_dir_path is None:
        raise ValueError("result_dir_path must be provided.")
    print(f"{model_name} has estimated outputs")
    anomalies = detect_anomalies(reconstruction_error, threshold)
    print(f"{model_name} reconstruction error calculated")
    df_score = create_dataframe(reconstruction_error, df_orig, df_top_3, pd.DataFrame(labels, columns=['PCA_Labels'])) # Ad
    all_anomalies = df_score[df_score.index.isin(df_orig[anomalies].index)].sort_values(by='anomaly_score', ascending=False
    print(f"{model_name} anomaly dataframe created")
    save_anomalies(all_anomalies, model_name, "All_Anomalies.csv", result_dir_path)
    print(f"{model_name} anomaly csv saved")
    df_filtered = filter_recent_anomalies(all_anomalies)
    # No index resetting here
    save_anomalies(df_filtered, model_name, "Recent_Anomalies.csv", result_dir_path)
    print(f"{model_name} recent anomaly csv saved\n")
```

Export to CSV

In [51]:
```
for key, value in models.items():
    reconstruction_error, top_3_max_diff_df = calculate_reconstruction_and_top_3_values(key, value, dataloader, df_scaled,
    detect_and_save_anomalies(key, value, dataloader, top_3_max_diff_df, labels, df_orig, 99.9, result_dir_path=result_dir_
```

A Jupyter widget could not be displayed because the widget state could not be found. This could happen if the kernel storing the widget is no longer available, or if the widget state was not saved in the notebook. You may be able to create the widget by running the appropriate cells.

```
model_1 has estimated outputs
model_1 reconstruction error calculated
model_1 anomaly dataframe created
model_1 anomaly csv saved
model_1 recent anomaly csv saved
```

A Jupyter widget could not be displayed because the widget state could not be found. This could happen if the kernel storing the widget is no longer available, or if the widget state was not saved in the notebook. You may be able to create the widget by running the appropriate cells.

```
model_2 has estimated outputs
model_2 reconstruction error calculated
model_2 anomaly dataframe created
model_2 anomaly csv saved
model_2 recent anomaly csv saved
```

A Jupyter widget could not be displayed because the widget state could not be found. This could happen if the kernel storing the widget is no longer available, or if the widget state was not saved in the notebook. You may be able to create the widget by running the appropriate cells.

```
model_3 has estimated outputs
model_3 reconstruction error calculated
model_3 anomaly dataframe created
model_3 anomaly csv saved
model_3 recent anomaly csv saved
```

A Jupyter widget could not be displayed because the widget state could not be found. This could happen if the kernel storing the widget is no longer available, or if the widget state was not saved in the notebook. You may be able to create the widget by running the appropriate cells.

```
model_4 has estimated outputs
model_4 reconstruction error calculated
model_4 anomaly dataframe created
model_4 anomaly csv saved
model_4 recent anomaly csv saved
```

In [ ]:
```
```