Attri-VAE for Interpretable Prediction of Myocardial Infarction Complications

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2025-04-23

```python
import torch
import torch.nn as nn
import torch.nn.functional as F
import torch.optim as optim
from torch.utils.data import Dataset, DataLoader, TensorDataset
from torch.optim.lr_scheduler import ReduceLROnPlateau

import numpy as np
import pandas as pd
import matplotlib.pyplot as plt
import seaborn as sns
from sklearn.preprocessing import StandardScaler
from sklearn.model_selection import train_test_split
from sklearn.metrics import roc_auc_score, average_precision_score, confusion_matrix
from sklearn.manifold import TSNE
from ucimlrepo import fetch_ucirepo

import os
import json
from pathlib import Path
from datetime import datetime
import logging
from tqdm.notebook import tqdm
import random
from collections import defaultdict
import copy

# Set up logging
logging.basicConfig(level=logging.INFO, format='%(asctime)s - %(levelname)s - %(message)s')
```

```python
logger = logging.getLogger()

# Set random seed for reproducibility
def set_seed(seed=42):
    random.seed(seed)
    np.random.seed(seed)
    torch.manual_seed(seed)
    if torch.cuda.is_available():
        torch.cuda.manual_seed(seed)
        torch.cuda.manual_seed_all(seed)
        torch.backends.cudnn.deterministic = True
        torch.backends.cudnn.benchmark = False

set_seed(42)

# Device configuration
device = torch.device('cuda' if torch.cuda.is_available() else 'cpu')
print(f"Using device: {device}")
```

```
Using device: cpu
```

```python
class MIDataset(Dataset):
    """
    Custom dataset for MI complications data with temporal structure
    """
    def __init__(
        self,
        X_timepoints,
        y,
        attributes,
        transform=None,
        target_transform=None
    ):
        """
        Initialize dataset

        Args:
            X_timepoints: Dictionary of feature dataframes for each timepoint
            y: Target array
            attributes: Clinical attributes for regularization
            transform: Optional transform to be applied to features
```

```
            target_transform: Optional transform to be applied to targets
        """
        self.X_timepoints = X_timepoints
        self.y = y
        self.attributes = attributes
        self.transform = transform
        self.target_transform = target_transform

        # Convert to tensors
        self.X_tensors = {
            tp: torch.FloatTensor(X.values)
            for tp, X in X_timepoints.items()
        }
        self.y_tensor = torch.FloatTensor(y.values)
        self.attributes_tensor = torch.FloatTensor(attributes.values)

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

    def __getitem__(self, idx):
        # Get features for each timepoint
        x_list = [self.X_tensors[tp][idx] for tp in sorted(self.X_tensors.keys())]

        # Get target and attributes
        y = self.y_tensor[idx]
        attributes = self.attributes_tensor[idx]

        # Apply transforms if specified
        if self.transform:
            x_list = [self.transform(x) for x in x_list]
        if self.target_transform:
            y = self.target_transform(y)

        return x_list, y, attributes

def load_mi_data():
    """
    Load and preprocess MI complications dataset

    Returns:
        X_timepoints: Dictionary of feature dataframes for each timepoint
        y: Target array
```

```
    attributes: Clinical attributes for regularization
"""
print("Loading MI Complications dataset from UCI repository...")
# Fetch the UCI MI complications dataset
mi = fetch_ucirepo(id=579)
X_full = mi.data.features
y_full = mi.data.targets

# Print dataset information
print(f"Dataset shape: {X_full.shape}")
print(f"Number of samples: {len(X_full)}")
print(f"Number of complications: {y_full.shape[1]}")

# Checking if dataset is loaded properly
if X_full is None or X_full.empty:
    raise ValueError("Failed to load features from UCI MI complications dataset")

# Create any-complication binary target
y = pd.Series((y_full.sum(axis=1) > 0).astype(int))
print(f"Positive samples (with complications): {y.sum()} ({y.mean()*100:.2f}%)")

# Define timepoints and their corresponding features
timepoints = {
    'admission': [col for col in X_full.columns if '_ADM' in col or col in ['AGE', 'SEX'
    '24h': [col for col in X_full.columns if '_24_' in col or '_24H' in col],
    '48h': [col for col in X_full.columns if '_48_' in col or '_48H' in col],
    '72h': [col for col in X_full.columns if '_72_' in col or '_72H' in col]
}

# Print timepoint information
for tp, cols in timepoints.items():
    print(f"Timepoint {tp}: {len(cols)} features")

# Create feature sets for each timepoint
X_timepoints = {}
for tp, cols in timepoints.items():
    if cols:  # Only process if we have columns for this timepoint
        X_tp = X_full[cols].copy()
        X_timepoints[tp] = X_tp

# Select clinical attributes for regularization
# These should be features that are clinically meaningful
```

```python
attribute_cols = [
    'AGE',
    'S_AD_ORIT',
    'D_AD_ORIT',
    'K_BLOOD',
    'L_BLOOD',
    'TIME_B_S'
]

# Filter to only include columns that exist in the dataset
attribute_cols = [col for col in attribute_cols if col in X_full.columns]
attributes = X_full[attribute_cols].copy()
print(f"Selected {len(attribute_cols)} clinical attributes: {attribute_cols}")

# Handle missing values
for tp, X in X_timepoints.items():
    # Check if any columns are fully NaN
    empty_cols = X.columns[X.isna().all()].tolist()
    if empty_cols:
        print(f"Warning: Dropping columns with all NaN values in {tp}: {empty_cols}")
        X.drop(columns=empty_cols, inplace=True)

    # Calculate percentage of missing values
    missing_pct = X.isna().mean().mean() * 100
    print(f"Timepoint {tp}: {missing_pct:.2f}% missing values")

    # Now fill remaining NaNs with column means
    X.fillna(X.mean(), inplace=True)

attributes.fillna(attributes.mean(), inplace=True)

# Scale features
scalers = {}
for tp, X in X_timepoints.items():
    if not X.empty:  # Only scale if we have data
        scaler = StandardScaler()
        X_timepoints[tp] = pd.DataFrame(
            scaler.fit_transform(X),
            columns=X.columns,
            index=X.index
        )
        scalers[tp] = scaler
```

```python
    # Scale attributes
    if not attributes.empty:
        attr_scaler = StandardScaler()
        attributes = pd.DataFrame(
            attr_scaler.fit_transform(attributes),
            columns=attributes.columns,
            index=attributes.index
        )

    print("Data preprocessing completed successfully.")
    return X_timepoints, y, attributes

def create_data_loaders(
    X_timepoints,
    y,
    attributes,
    batch_size=32,
    val_size=0.2,
    test_size=0.1,
    random_state=42
):
    """
    Create train, validation, and test data loaders

    Args:
        X_timepoints: Dictionary of feature dataframes for each timepoint
        y: Target array
        attributes: Clinical attributes for regularization
        batch_size: Batch size for data loaders
        val_size: Proportion of data to use for validation
        test_size: Proportion of data to use for testing
        random_state: Random seed for reproducibility

    Returns:
        train_loader: DataLoader for training data
        val_loader: DataLoader for validation data
        test_loader: DataLoader for test data
    """
    print("Creating train/val/test splits...")
    # First split into train+val and test
    train_val_idx, test_idx = train_test_split(
        np.arange(len(y)),
```

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        test_size=test_size,
        random_state=random_state,
        stratify=y
    )

    # Then split train+val into train and val
    train_idx, val_idx = train_test_split(
        train_val_idx,
        test_size=val_size/(1-test_size),
        random_state=random_state,
        stratify=y.iloc[train_val_idx]
    )

    print(f"Train set: {len(train_idx)} samples ({y.iloc[train_idx].mean()*100:.2f}% positive
    print(f"Validation set: {len(val_idx)} samples ({y.iloc[val_idx].mean()*100:.2f}% positi
    print(f"Test set: {len(test_idx)} samples ({y.iloc[test_idx].mean()*100:.2f}% positive)")

    # Create datasets
    train_dataset = MIDataset(
        {tp: X.iloc[train_idx] for tp, X in X_timepoints.items()},
        y.iloc[train_idx],
        attributes.iloc[train_idx]
    )

    val_dataset = MIDataset(
        {tp: X.iloc[val_idx] for tp, X in X_timepoints.items()},
        y.iloc[val_idx],
        attributes.iloc[val_idx]
    )

    test_dataset = MIDataset(
        {tp: X.iloc[test_idx] for tp, X in X_timepoints.items()},
        y.iloc[test_idx],
        attributes.iloc[test_idx]
    )

    # Create data loaders with num_workers=0 to avoid multiprocessing issues in Jupyter
    train_loader = DataLoader(
        train_dataset,
        batch_size=batch_size,
        shuffle=True,
        num_workers=0  # Changed from 4 to 0
```

```
    )

    val_loader = DataLoader(
        val_dataset,
        batch_size=batch_size,
        shuffle=False,
        num_workers=0  # Changed from 4 to 0
    )

    test_loader = DataLoader(
        test_dataset,
        batch_size=batch_size,
        shuffle=False,
        num_workers=0  # Changed from 4 to 0
    )

    print("Data loaders created successfully.")
    return train_loader, val_loader, test_loader

# Load and prepare data
X_timepoints, y, attributes = load_mi_data()
train_loader, val_loader, test_loader = create_data_loaders(X_timepoints, y, attributes)

# Extract feature dimensions for model configuration
input_dims = [X.shape[1] for X in X_timepoints.values()]
attribute_dims = {attr: i for i, attr in enumerate(attributes.columns)}
print(f"Input dimensions: {input_dims}")
print(f"Attribute dimensions: {attribute_dims}")
```

```
Loading MI Complications dataset from UCI repository...
Dataset shape: (1700, 111)
Number of samples: 1700
Number of complications: 12
Positive samples (with complications): 1037 (61.00%)
Timepoint admission: 3 features
Timepoint 24h: 0 features
Timepoint 48h: 0 features
Timepoint 72h: 0 features
Selected 6 clinical attributes: ['AGE', 'S_AD_ORIT', 'D_AD_ORIT', 'K_BLOOD', 'L_BLOOD', 'TIM
Timepoint admission: 2.63% missing values
Data preprocessing completed successfully.
Creating train/val/test splits...
```

```
Train set: 1190 samples (61.01% positive)
Validation set: 340 samples (60.88% positive)
Test set: 170 samples (61.18% positive)
Data loaders created successfully.
Input dimensions: [3]
Attribute dimensions: {'AGE': 0, 'S_AD_ORIT': 1, 'D_AD_ORIT': 2, 'K_BLOOD': 3, 'L_BLOOD': 4,
```

```python
class MedicalSafetyLayer(nn.Module):
    """
    Layer to enforce physiological ranges for outputs
    """
    def __init__(self, feature_ranges=None):
        """
        Initialize layer with physiological ranges

        Args:
            feature_ranges: Dictionary mapping feature names to (min, max) range tuples
        """
        super(MedicalSafetyLayer, self).__init__()
        self.feature_ranges = feature_ranges or {
            # Systolic BP (mmHg)
            'S_AD': (80, 180),
            # Diastolic BP (mmHg)
            'D_AD': (40, 120),
            # Heart rate (bpm)
            'RATE_AD': (40, 180),
            # Body temperature (°C)
            'TEMP_AD': (35, 41),
            # Potassium (mmol/L)
            'K_BLOOD': (3.0, 6.0),
            # Sodium (mmol/L)
            'Na_BLOOD': (130, 150),
            # White blood cells (10^9/L)
            'L_BLOOD': (4.0, 25.0)
        }

    def forward(self, x, feature_names=None):
        """
        Apply safety constraints to outputs

        Args:
            x: Input tensor
```

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            feature_names: List of feature names corresponding to dimensions

        Returns:
            x_safe: Output tensor with values within safe ranges
            safety_loss: Loss penalizing values outside physiological ranges
        """
        # If feature names not provided, return unchanged
        if feature_names is None:
            return x, None

        # Initialize loss
        safety_loss = 0.0

        # Apply safety constraints
        for i, name in enumerate(feature_names):
            for key, (min_val, max_val) in self.feature_ranges.items():
                if key in name:
                    # Calculate penalty for out-of-range values
                    below_min = F.relu(min_val - x[:, i])
                    above_max = F.relu(x[:, i] - max_val)
                    penalty = below_min + above_max
                    safety_loss += torch.mean(penalty)

        return x, safety_loss

class GroupLatentToTimepoint(nn.Module):
    """
    Group-sparse latent-to-timepoint transformation as in oi-VAE
    """
    def __init__(self, latent_dim, hidden_dim, timepoints):
        super(GroupLatentToTimepoint, self).__init__()
        self.latent_dim = latent_dim
        self.hidden_dim = hidden_dim
        self.timepoints = timepoints

        # Group-specific latent-to-timepoint matrices (one per timepoint)
        # These will be subject to group sparsity regularization
        self.W = nn.ParameterDict({
            tp: nn.Parameter(torch.randn(hidden_dim, latent_dim) * 0.01)
            for tp in timepoints
        })
```

```python
    def forward(self, z):
        """
        Transform latent vector with group-specific matrices

        Args:
            z: Latent vector [batch_size, latent_dim]

        Returns:
            outputs: Dictionary of timepoint-specific transformed vectors
        """
        outputs = {}
        for tp in self.timepoints:
            # Apply group-specific transformation
            outputs[tp] = F.linear(z, self.W[tp])
        return outputs

    def get_group_norms(self):
        """
        Compute the L2 norm of each column in each group matrix
        Used for proximal gradient updates and visualization

        Returns:
            Dictionary of norms per timepoint and latent dimension
        """
        norms = {}
        for tp in self.timepoints:
            # Compute column-wise L2 norms: [latent_dim]
            norms[tp] = torch.norm(self.W[tp], dim=0)
        return norms

    def apply_proximal_update(self, lr, lambda_reg):
        """
        Apply proximal gradient update for group sparsity

        Args:
            lr: Learning rate
            lambda_reg: Regularization strength
        """
        with torch.no_grad():
            for tp in self.timepoints:
                # Compute column-wise L2 norms
                norms = torch.norm(self.W[tp], dim=0, keepdim=True)
```

```
                # Apply proximal operator: shrink columns toward zero
                # max(0, 1 - lambda*lr/norm) * w
                scale = torch.clamp(1 - lambda_reg * lr / (norms + 1e-8), min=0.0)
                self.W[tp].mul_(scale)

class GroupInterpretableVAE(nn.Module):
    """
    Group-structured interpretable VAE for MI complications prediction with attribute regula
    """
    def __init__(
        self,
        input_dims,
        timepoint_names,
        latent_dim=32,
        embed_dim=16,
        hidden_dim=64,
        attribute_dims=None,
        medical_safety=True
    ):
        """
        Initialize model

        Args:
            input_dims: List of input dimensions for each timepoint
            timepoint_names: List of timepoint names (e.g., 'admission', '24h')
            latent_dim: Dimension of the latent space
            embed_dim: Dimension of time embeddings
            hidden_dim: Dimension of hidden layers
            attribute_dims: Dictionary mapping attribute name to latent dimension index
            medical_safety: Whether to enforce medical safety constraints
        """
        super(GroupInterpretableVAE, self).__init__()

        self.input_dims = input_dims if isinstance(input_dims, list) else list(input_dims)
        self.timepoint_names = timepoint_names
        self.latent_dim = latent_dim
        self.embed_dim = embed_dim
        self.hidden_dim = hidden_dim
        self.attribute_dims = attribute_dims or {}
        self.medical_safety = medical_safety

        # Time embeddings (one for each timepoint)
```

```
        self.time_embeddings = nn.Embedding(len(input_dims), embed_dim)

        # Encoders for each timepoint
        self.encoders = nn.ModuleList([
            nn.Sequential(
                nn.Linear(dim + embed_dim, hidden_dim),
                nn.BatchNorm1d(hidden_dim),
                nn.ReLU(),
                nn.Linear(hidden_dim, hidden_dim // 2),
                nn.BatchNorm1d(hidden_dim // 2),
                nn.ReLU()
            ) for dim in input_dims
        ])

        # Latent projectors (mu and logvar)
        encoder_output_dim = (hidden_dim // 2) * len(input_dims)
        self.mu_projector = nn.Linear(encoder_output_dim, latent_dim)
        self.logvar_projector = nn.Linear(encoder_output_dim, latent_dim)

        # Group-specific latent-to-timepoint transformation with sparsity
        self.group_transform = GroupLatentToTimepoint(latent_dim, hidden_dim, timepoint_names

        # Integration module
        self.integration = nn.Sequential(
            nn.Linear(latent_dim, latent_dim),
            nn.BatchNorm1d(latent_dim),
            nn.ReLU()
        )

        # Attribute predictor for regularization
        self.attribute_predictor = nn.Linear(latent_dim, len(attribute_dims))

        # Classifier for complications prediction
        self.classifier = nn.Sequential(
            nn.Linear(latent_dim, hidden_dim // 2),
            nn.BatchNorm1d(hidden_dim // 2),
            nn.ReLU(),
            nn.Dropout(0.2),
            nn.Linear(hidden_dim // 2, hidden_dim // 4),
            nn.BatchNorm1d(hidden_dim // 4),
            nn.ReLU(),
            nn.Dropout(0.2),
```

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            nn.Linear(hidden_dim // 4, 1)
        )

        # Decoders for each timepoint
        self.decoders = nn.ModuleDict({
            tp: nn.Sequential(
                nn.Linear(hidden_dim + embed_dim, hidden_dim),
                nn.BatchNorm1d(hidden_dim),
                nn.ReLU(),
                nn.Linear(hidden_dim, dim)
            ) for tp, dim in zip(timepoint_names, input_dims)
        })

        # Medical safety layer
        if medical_safety:
            self.safety_layer = MedicalSafetyLayer()

        # Loss functions
        self.mse_loss = nn.MSELoss(reduction='mean')
        self.bce_loss = nn.BCEWithLogitsLoss(reduction='mean')

    def encode(self, x_list, attributes=None):
        """
        Encode a list of inputs from different timepoints

        Args:
            x_list: List of input tensors
            attributes: Clinical attributes tensor

        Returns:
            mu: Mean vector
            logvar: Log variance vector
        """
        batch_size = x_list[0].size(0)
        encodings = []

        # Generate time embeddings
        time_indices = torch.arange(len(self.encoders), device=x_list[0].device)
        time_embeds = self.time_embeddings(time_indices)

        # Encode each timepoint with its time embedding
        for i, (x, encoder) in enumerate(zip(x_list, self.encoders)):
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            # Add time embedding to input
            time_embed = time_embeds[i].expand(batch_size, -1)
            x_t = torch.cat([x, time_embed], dim=1)

            # Encode
            h = encoder(x_t)
            encodings.append(h)

        # Concatenate all encodings
        concat_encoding = torch.cat(encodings, dim=1)

        # Project to latent space
        mu = self.mu_projector(concat_encoding)
        logvar = self.logvar_projector(concat_encoding)

        return mu, logvar

    def reparameterize(self, mu, logvar):
        """
        Reparameterization trick to sample from distribution

        Args:
            mu: Mean vector
            logvar: Log variance vector

        Returns:
            z: Sampled latent vector
        """
        std = torch.exp(0.5 * logvar)
        eps = torch.randn_like(std)
        return mu + eps * std

    def decode(self, z):
        """
        Decode latent representation using group-sparse transformations

        Args:
            z: Latent vector

        Returns:
            recon_list: List of reconstructions for each timepoint
            safety_loss: Medical safety loss if enabled
```

```
        """
        batch_size = z.size(0)
        recon_list = []
        safety_loss = None

        # Apply group-specific latent-to-timepoint transformations with sparsity
        transformed = self.group_transform(z)

        # Generate time embeddings
        time_indices = torch.arange(len(self.timepoint_names), device=z.device)
        time_embeds = self.time_embeddings(time_indices)

        # Decode each timepoint
        for i, tp in enumerate(self.timepoint_names):
            # Add time embedding
            time_embed = time_embeds[i].expand(batch_size, -1)
            h = torch.cat([transformed[tp], time_embed], dim=1)

            # Decode
            x_recon = self.decoders[tp](h)

            # Apply medical safety constraints if enabled
            if self.medical_safety:
                x_recon, time_safety_loss = self.safety_layer(x_recon)
                if time_safety_loss is not None:
                    if safety_loss is None:
                        safety_loss = time_safety_loss
                    else:
                        safety_loss += time_safety_loss

            recon_list.append(x_recon)

        return recon_list, safety_loss

    def predict_attributes(self, z):
        """
        Predict attributes from latent vector for regularization

        Args:
            z: Latent vector

        Returns:
```

```
        attr_pred: Predicted attributes
    """
    return self.attribute_predictor(z)

def forward(self, x_list, attributes=None):
    """
    Forward pass

    Args:
        x_list: List of input tensors
        attributes: Clinical attributes tensor

    Returns:
        recon_list: List of reconstructions
        mu: Mean vector
        logvar: Log variance vector
        attr_pred: Predicted attributes
        y_pred: Predicted complication probability
        safety_loss: Medical safety loss if enabled
    """
    # Encode
    mu, logvar = self.encode(x_list, attributes)

    # Sample latent vector
    z = self.reparameterize(mu, logvar)

    # Integrate latent representation
    z = self.integration(z)

    # Predict attributes
    attr_pred = self.predict_attributes(z)

    # Predict complications
    y_pred = self.classifier(z)

    # Decode
    recon_list, safety_loss = self.decode(z)

    return recon_list, mu, logvar, attr_pred, y_pred, safety_loss

def compute_losses(self, outputs, targets, attributes):
    """
```

```
        Compute all loss components

        Args:
            outputs: Model outputs (recon_list, mu, logvar, attr_pred, y_pred, safety_loss)
            targets: Target values (x_list, y, _)
            attributes: Clinical attributes

        Returns:
            total_loss: Total weighted loss
            loss_dict: Dictionary of individual loss components
        """
        # Unpack outputs
        reconstructions, mu, logvar, pred_attributes, y_pred, safety_loss = outputs
        x_list, y, _ = targets

        # Ensure y and y_pred have the same shape
        y = y.view(-1, 1) if y_pred.shape[-1] == 1 else y

        # 1. Reconstruction loss (MSE)
        recon_loss = 0
        for i, (x, recon) in enumerate(zip(x_list, reconstructions)):
            recon_loss += self.mse_loss(recon, x)
        recon_loss /= len(x_list)

        # 2. KL divergence loss
        kl_loss = -0.5 * torch.mean(1 + logvar - mu.pow(2) - logvar.exp())

        # 3. Attribute regularization loss
        attr_loss = self.mse_loss(pred_attributes, attributes)

        # 4. Classification loss for complications
        cls_loss = self.bce_loss(y_pred, y)

        # 5. Group sparsity loss (computed during optimization)

        # Total loss with weighting
        total_loss = recon_loss + self.beta * kl_loss + self.gamma * attr_loss + cls_loss

        # Add medical safety loss if available
        if safety_loss is not None:
            total_loss += self.delta * safety_loss
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        # Return individual losses for logging
        loss_dict = {
            'loss': total_loss.item(),
            'recon_loss': recon_loss.item(),
            'kl_loss': kl_loss.item(),
            'attr_loss': attr_loss.item(),
            'cls_loss': cls_loss.item(),
        }

        if safety_loss is not None:
            loss_dict['safety_loss'] = safety_loss.item()

        return total_loss, loss_dict

    def apply_proximal_update(self, lr, lambda_reg):
        """
        Apply proximal gradient update for group sparsity

        Args:
            lr: Learning rate
            lambda_reg: Regularization strength
        """
        self.group_transform.apply_proximal_update(lr, lambda_reg)

    def get_group_sparsity_visualization(self):
        """
        Get matrix of group norms for visualization

        Returns:
            Group norm matrix for heatmap visualization
        """
        norms = self.group_transform.get_group_norms()

        # Convert to numpy for visualization
        norm_matrix = np.zeros((len(self.timepoint_names), self.latent_dim))
        for i, tp in enumerate(self.timepoint_names):
            norm_matrix[i] = norms[tp].cpu().detach().numpy()

        return norm_matrix
```

```python
class TensorboardCallback:
    """Callback for logging metrics to TensorBoard during training"""
```

```python
    def __init__(self, writer):
        self.writer = writer
        self.step = 0

    def on_epoch_end(self, epoch, train_metrics, val_metrics):
        """Log metrics at the end of each epoch"""
        # Log training metrics
        for k, v in train_metrics.items():
            if isinstance(v, (int, float)):
                self.writer.add_scalar(f'train/{k}', v, epoch)

        # Log validation metrics
        for k, v in val_metrics.items():
            if isinstance(v, (int, float)):
                self.writer.add_scalar(f'val/{k}', v, epoch)

        # Log learning rate
        for i, param_group in enumerate(self.optimizer.param_groups):
            self.writer.add_scalar(f'lr/group_{i}', param_group['lr'], epoch)

    def set_optimizer(self, optimizer):
        """Set the optimizer for learning rate tracking"""
        self.optimizer = optimizer

class GroupInterpretableVAETrainer:
    """
    Trainer for Group Interpretable VAE with collapsed variational inference
    """
    def __init__(
        self,
        model,
        train_loader,
        val_loader,
        device,
        lr=1e-3,
        weight_decay=1e-5,
        beta=1.0,        # KL weight
        gamma=0.1,       # Attribute regularization weight
        delta=0.1,       # Medical safety weight
        lambda_reg=1.0,  # Group sparsity weight
        callbacks=None
    ):
```

```
        """
        Initialize trainer

        Args:
            model: GroupInterpretableVAE model
            train_loader: DataLoader for training data
            val_loader: DataLoader for validation data
            device: Device to use (cuda or cpu)
            lr: Learning rate
            weight_decay: Weight decay
            beta: KL divergence weight
            gamma: Attribute regularization weight
            delta: Medical safety weight
            lambda_reg: Group sparsity regularization strength
            callbacks: List of callbacks for training events
        """
        self.model = model.to(device)
        self.train_loader = train_loader
        self.val_loader = val_loader
        self.device = device
        self.lr = lr
        self.lambda_reg = lambda_reg

        # Set loss weights
        self.model.beta = beta
        self.model.gamma = gamma
        self.model.delta = delta

        # Initialize optimizer
        self.optimizer = optim.Adam(
            model.parameters(),
            lr=lr,
            weight_decay=weight_decay
        )

        # Initialize learning rate scheduler
        self.scheduler = ReduceLROnPlateau(
            self.optimizer,
            mode='min',
            factor=0.5,
            patience=5
        )
```

```
        # Callbacks
        self.callbacks = callbacks or []

        # Set optimizer in callbacks
        for callback in self.callbacks:
            if hasattr(callback, 'set_optimizer'):
                callback.set_optimizer(self.optimizer)

    def train_epoch(self, epoch):
        """
        Train model for one epoch with collapsed variational inference

        Args:
            epoch: Current epoch number

        Returns:
            avg_loss: Average loss for the epoch
            metrics: Dictionary of metrics
        """
        self.model.train()
        running_loss = 0.0
        loss_dict_sum = defaultdict(float)
        predictions = []
        targets = []

        # Create progress bar
        pbar = tqdm(self.train_loader, desc=f'Epoch {epoch+1} [Train]')

        for batch_idx, (x_list, y, attributes) in enumerate(pbar):
            # Move data to device
            x_list = [x.to(self.device) for x in x_list]
            y = y.to(self.device)
            attributes = attributes.to(self.device)

            # Zero gradients
            self.optimizer.zero_grad()

            # Forward pass
            outputs = self.model(x_list, attributes)

            # Compute loss
            loss, batch_loss_dict = self.model.compute_losses(outputs, (x_list, y, attribute
```

```python
            # Backward pass
            loss.backward()

            # Update weights with standard gradient descent
            self.optimizer.step()

            # Apply proximal update for group sparsity
            self.model.apply_proximal_update(self.lr, self.lambda_reg)

            # Update running loss
            running_loss += loss.item()
            for k, v in batch_loss_dict.items():
                loss_dict_sum[k] += v

            # Update progress bar
            pbar.set_postfix({'loss': loss.item()})

            # Store predictions for metrics
            y_pred = outputs[4]
            predictions.append(y_pred.detach().cpu().numpy())
            targets.append(y.detach().cpu().numpy())

        # Concatenate predictions and targets
        predictions = np.concatenate(predictions)
        targets = np.concatenate(targets)

        # Reshape for metrics calculation
        predictions = predictions.reshape(-1)
        targets = targets.reshape(-1)

        # Calculate metrics
        metrics = {}
        for k, v in loss_dict_sum.items():
            metrics[k] = v / len(self.train_loader)

        # Calculate classification metrics
        try:
            metrics['auroc'] = roc_auc_score(targets, predictions)
            metrics['auprc'] = average_precision_score(targets, predictions)
        except Exception as e:
            print(f"Error calculating metrics: {e}")
            metrics['auroc'] = 0.0
```

```python
            metrics['auprc'] = 0.0

        return metrics['loss'], metrics

    def validate(self, dataloader=None):
        """
        Validate model on validation set

        Args:
            dataloader: DataLoader to use for validation (default: self.val_loader)

        Returns:
            avg_loss: Average loss for validation
            metrics: Dictionary of metrics
        """
        if dataloader is None:
            dataloader = self.val_loader

        self.model.eval()
        running_loss = 0.0
        loss_dict_sum = defaultdict(float)
        predictions = []
        targets = []

        with torch.no_grad():
            # Create progress bar
            pbar = tqdm(dataloader, desc='Validation')

            for batch_idx, (x_list, y, attributes) in enumerate(pbar):
                # Move data to device
                x_list = [x.to(self.device) for x in x_list]
                y = y.to(self.device)
                attributes = attributes.to(self.device)

                # Forward pass
                outputs = self.model(x_list, attributes)

                # Compute loss
                loss, batch_loss_dict = self.model.compute_losses(outputs, (x_list, y, attri

                # Update running loss
                running_loss += loss.item()
```

```
            for k, v in batch_loss_dict.items():
                loss_dict_sum[k] += v

            # Update progress bar
            pbar.set_postfix({'loss': loss.item()})

            # Store predictions for metrics
            y_pred = outputs[4]
            predictions.append(y_pred.detach().cpu().numpy())
            targets.append(y.detach().cpu().numpy())

    # Concatenate predictions and targets
    predictions = np.concatenate(predictions)
    targets = np.concatenate(targets)

    # Reshape for metrics calculation
    predictions = predictions.reshape(-1)
    targets = targets.reshape(-1)

    # Calculate metrics
    metrics = {}
    for k, v in loss_dict_sum.items():
        metrics[k] = v / len(dataloader)

    # Calculate classification metrics
    try:
        metrics['auroc'] = roc_auc_score(targets, predictions)
        metrics['auprc'] = average_precision_score(targets, predictions)
    except Exception as e:
        print(f"Error calculating metrics: {e}")
        metrics['auroc'] = 0.0
        metrics['auprc'] = 0.0

    return metrics

def train(self, n_epochs=100, early_stopping_patience=10, checkpoint_dir="./checkpoints"
    """
    Train the model with early stopping

    Args:
        n_epochs: Maximum number of epochs to train
        early_stopping_patience: Number of epochs to wait for improvement before stoppin
```

```
            checkpoint_dir: Directory to save model checkpoints

        Returns:
            history: Dictionary of training and validation metrics
            best_model: Best model state dict
        """
        # Create checkpoint directory if it doesn't exist
        os.makedirs(checkpoint_dir, exist_ok=True)

        # Initialize variables for training
        best_val_loss = float('inf')
        best_model_state = None
        patience_counter = 0
        history = {'train': [], 'val': []}

        print(f"Starting training for {n_epochs} epochs with early stopping patience {early_s

        for epoch in range(n_epochs):
            # Train for one epoch
            train_loss, train_metrics = self.train_epoch(epoch)

            # Validate
            val_metrics = self.validate()
            val_loss = val_metrics['loss']

            # Update learning rate scheduler
            self.scheduler.step(val_loss)

            # Save metrics in history
            history['train'].append(train_metrics)
            history['val'].append(val_metrics)

            # Print epoch summary
            print(f"Epoch {epoch+1}/{n_epochs} - "
                f"Train Loss: {train_loss:.4f}, "
                f"Val Loss: {val_loss:.4f}, "
                f"Train AUROC: {train_metrics.get('auroc', 0):.4f}, "
                f"Val AUROC: {val_metrics.get('auroc', 0):.4f}")

            # Call callbacks
            for callback in self.callbacks:
                if hasattr(callback, 'on_epoch_end'):
```

```python
                callback.on_epoch_end(epoch, train_metrics, val_metrics)

        # Check for improvement
        if val_loss < best_val_loss:
            best_val_loss = val_loss
            best_model_state = copy.deepcopy(self.model.state_dict())
            patience_counter = 0

            # Save the best model
            checkpoint_path = os.path.join(checkpoint_dir, f"best_model.pt")
            torch.save({
                'epoch': epoch,
                'model_state_dict': self.model.state_dict(),
                'optimizer_state_dict': self.optimizer.state_dict(),
                'train_metrics': train_metrics,
                'val_metrics': val_metrics,
            }, checkpoint_path)
            print(f"Saved best model at epoch {epoch+1} with val_loss: {val_loss:.4f}")
        else:
            patience_counter += 1
            if patience_counter >= early_stopping_patience:
                print(f"Early stopping triggered after {epoch+1} epochs")
                break

    # Load the best model
    if best_model_state is not None:
        self.model.load_state_dict(best_model_state)

    return history, self.model
```

```python
def plot_training_history(history):
    """
    Plot training and validation metrics

    Args:
        history: Dictionary of training and validation metrics from trainer
    """
    # Convert history to DataFrame for easier plotting
    epochs = range(1, len(history['train']) + 1)
    metrics = ['loss', 'recon_loss', 'kl_loss', 'attr_loss', 'cls_loss', 'auroc', 'auprc']

    plt.figure(figsize=(15, 12))
```

```
    for i, metric in enumerate(metrics):
        if metric not in history['train'][0]:
            continue

        plt.subplot(3, 3, i+1)

        # Get train and val values for the metric
        train_values = [epoch_metrics.get(metric, 0) for epoch_metrics in history['train']]
        val_values = [epoch_metrics.get(metric, 0) for epoch_metrics in history['val']]

        plt.plot(epochs, train_values, 'b-', label=f'Train {metric}')
        plt.plot(epochs, val_values, 'r-', label=f'Val {metric}')

        plt.title(f'{metric} vs. Epochs')
        plt.xlabel('Epochs')
        plt.ylabel(metric)
        plt.legend()

        # Highlight best epoch (lowest val loss or highest val auroc)
        if metric == 'loss':
            best_epoch = np.argmin(val_values) + 1
            plt.axvline(x=best_epoch, color='g', linestyle='--')
            plt.text(best_epoch + 0.1, min(train_values), f'Best epoch: {best_epoch}')
        elif metric == 'auroc':
            best_epoch = np.argmax(val_values) + 1
            plt.axvline(x=best_epoch, color='g', linestyle='--')
            plt.text(best_epoch + 0.1, max(val_values), f'Best epoch: {best_epoch}')

    plt.tight_layout()
    plt.show()

def visualize_latent_space(model, test_loader, device, plot_type='tsne'):
    """
    Visualize the latent space using t-SNE or PCA

    Args:
        model: Trained model
        test_loader: DataLoader for test data
        device: Device to use
        plot_type: 'tsne' or 'pca'
    """
    model.eval()
```

```python
latent_vectors = []
labels = []

with torch.no_grad():
    for x_list, y, attributes in test_loader:
        # Move data to device
        x_list = [x.to(device) for x in x_list]

        # Get latent representation (mu)
        mu, _ = model.encode(x_list)

        # Store latent vectors and labels
        latent_vectors.append(mu.cpu().numpy())
        labels.append(y.cpu().numpy())

# Concatenate batches
latent_vectors = np.concatenate(latent_vectors, axis=0)
labels = np.concatenate(labels, axis=0)

# Apply dimensionality reduction
if plot_type == 'tsne':
    reducer = TSNE(n_components=2, random_state=42)
    reduced_data = reducer.fit_transform(latent_vectors)
    title = 't-SNE Visualization of Latent Space'
else:  # pca
    from sklearn.decomposition import PCA
    reducer = PCA(n_components=2, random_state=42)
    reduced_data = reducer.fit_transform(latent_vectors)
    title = 'PCA Visualization of Latent Space'

# Plot
plt.figure(figsize=(10, 8))
scatter = plt.scatter(reduced_data[:, 0], reduced_data[:, 1], c=labels, alpha=0.6,
                      cmap='coolwarm', edgecolors='w', s=100)

plt.colorbar(scatter, label='Complication')
plt.title(title)
plt.xlabel('Dimension 1')
plt.ylabel('Dimension 2')
plt.grid(True, alpha=0.3)
plt.tight_layout()
plt.show()
```

```python
def visualize_group_sparsity(model):
    """
    Visualize the group sparsity patterns

    Args:
        model: Trained model
    """
    # Get group sparsity matrix
    norm_matrix = model.get_group_sparsity_visualization()

    plt.figure(figsize=(12, 8))
    sns.heatmap(norm_matrix, cmap='viridis',
                xticklabels=[f'z{i+1}' for i in range(model.latent_dim)],
                yticklabels=model.timepoint_names,
                annot=False, cbar=True)

    plt.title('Group Sparsity Pattern')
    plt.xlabel('Latent Dimensions')
    plt.ylabel('Timepoints')
    plt.tight_layout()
    plt.show()

    # Analyze which latent dimensions are active for each timepoint
    for i, tp in enumerate(model.timepoint_names):
        active_dims = np.where(norm_matrix[i] > 0.1)[0]  # Threshold can be adjusted
        print(f"Timepoint {tp} is influenced by latent dimensions: {list(active_dims + 1)}")

def visualize_attribute_regularization(model, test_loader, device):
    """
    Visualize how latent dimensions correspond to clinical attributes

    Args:
        model: Trained model
        test_loader: DataLoader for test data
        device: Device to use
    """
    model.eval()
    latent_vectors = []
    all_attributes = []

    with torch.no_grad():
        for x_list, _, attributes in test_loader:
```

```
            # Move data to device
            x_list = [x.to(device) for x in x_list]

            # Get latent representation (mu)
            mu, _ = model.encode(x_list)

            # Store latent vectors and attributes
            latent_vectors.append(mu.cpu().numpy())
            all_attributes.append(attributes.cpu().numpy())

    # Concatenate batches
    latent_vectors = np.concatenate(latent_vectors, axis=0)
    all_attributes = np.concatenate(all_attributes, axis=0)

    # Calculate correlations between latent dimensions and attributes
    corr_matrix = np.zeros((model.latent_dim, all_attributes.shape[1]))

    for i in range(model.latent_dim):
        for j in range(all_attributes.shape[1]):
            corr = np.corrcoef(latent_vectors[:, i], all_attributes[:, j])[0, 1]
            corr_matrix[i, j] = corr

    # Plot correlation heatmap
    plt.figure(figsize=(10, 8))
    sns.heatmap(corr_matrix, cmap='coolwarm', center=0,
                xticklabels=list(model.attribute_dims.keys()),
                yticklabels=[f'z{i+1}' for i in range(model.latent_dim)],
                annot=True, fmt='.2f')

    plt.title('Correlation between Latent Dimensions and Clinical Attributes')
    plt.xlabel('Clinical Attributes')
```

```
def plot_training_history(history):
    """
    Plot training and validation metrics

    Args:
        history: Dictionary of training and validation metrics from trainer
    """
    # Convert history to DataFrame for easier plotting
    epochs = range(1, len(history['train']) + 1)
    metrics = ['loss', 'recon_loss', 'kl_loss', 'attr_loss', 'cls_loss', 'auroc', 'auprc']
```

```python
    plt.figure(figsize=(15, 12))

    for i, metric in enumerate(metrics):
        if metric not in history['train'][0]:
            continue

        plt.subplot(3, 3, i+1)

        # Get train and val values for the metric
        train_values = [epoch_metrics.get(metric, 0) for epoch_metrics in history['train']]
        val_values = [epoch_metrics.get(metric, 0) for epoch_metrics in history['val']]

        plt.plot(epochs, train_values, 'b-', label=f'Train {metric}')
        plt.plot(epochs, val_values, 'r-', label=f'Val {metric}')

        plt.title(f'{metric} vs. Epochs')
        plt.xlabel('Epochs')
        plt.ylabel(metric)
        plt.legend()

        # Highlight best epoch (lowest val loss or highest val auroc)
        if metric == 'loss':
            best_epoch = np.argmin(val_values) + 1
            plt.axvline(x=best_epoch, color='g', linestyle='--')
            plt.text(best_epoch + 0.1, min(train_values), f'Best epoch: {best_epoch}')
        elif metric == 'auroc':
            best_epoch = np.argmax(val_values) + 1
            plt.axvline(x=best_epoch, color='g', linestyle='--')
            plt.text(best_epoch + 0.1, max(val_values), f'Best epoch: {best_epoch}')

    plt.tight_layout()
    plt.show()

def visualize_latent_space(model, test_loader, device, plot_type='tsne'):
    """
    Visualize the latent space using t-SNE or PCA

    Args:
        model: Trained model
        test_loader: DataLoader for test data
        device: Device to use
        plot_type: 'tsne' or 'pca'
```

```
"""
model.eval()
latent_vectors = []
labels = []

with torch.no_grad():
    for x_list, y, attributes in test_loader:
        # Move data to device
        x_list = [x.to(device) for x in x_list]

        # Get latent representation (mu)
        mu, _ = model.encode(x_list)

        # Store latent vectors and labels
        latent_vectors.append(mu.cpu().numpy())
        labels.append(y.cpu().numpy())

# Concatenate batches
latent_vectors = np.concatenate(latent_vectors, axis=0)
labels = np.concatenate(labels, axis=0)

# Apply dimensionality reduction
if plot_type == 'tsne':
    reducer = TSNE(n_components=2, random_state=42)
    reduced_data = reducer.fit_transform(latent_vectors)
    title = 't-SNE Visualization of Latent Space'
else:  # pca
    from sklearn.decomposition import PCA
    reducer = PCA(n_components=2, random_state=42)
    reduced_data = reducer.fit_transform(latent_vectors)
    title = 'PCA Visualization of Latent Space'

# Plot
plt.figure(figsize=(10, 8))
scatter = plt.scatter(reduced_data[:, 0], reduced_data[:, 1], c=labels, alpha=0.6,
                      cmap='coolwarm', edgecolors='w', s=100)

plt.colorbar(scatter, label='Complication')
plt.title(title)
plt.xlabel('Dimension 1')
plt.ylabel('Dimension 2')
plt.grid(True, alpha=0.3)
```

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

def visualize_group_sparsity(model):
    """
    Visualize the group sparsity patterns

    Args:
        model: Trained model
    """
    # Get group sparsity matrix
    norm_matrix = model.get_group_sparsity_visualization()

    plt.figure(figsize=(12, 8))
    sns.heatmap(norm_matrix, cmap='viridis',
                xticklabels=[f'z{i+1}' for i in range(model.latent_dim)],
                yticklabels=model.timepoint_names,
                annot=False, cbar=True)

    plt.title('Group Sparsity Pattern')
    plt.xlabel('Latent Dimensions')
    plt.ylabel('Timepoints')
    plt.tight_layout()
    plt.show()

    # Analyze which latent dimensions are active for each timepoint
    for i, tp in enumerate(model.timepoint_names):
        active_dims = np.where(norm_matrix[i] > 0.1)[0]  # Threshold can be adjusted
        print(f"Timepoint {tp} is influenced by latent dimensions: {list(active_dims + 1)}")

def visualize_attribute_regularization(model, test_loader, device):
    """
    Visualize how latent dimensions correspond to clinical attributes

    Args:
        model: Trained model
        test_loader: DataLoader for test data
        device: Device to use
    """
    model.eval()
    latent_vectors = []
    all_attributes = []
```

```
with torch.no_grad():
    for x_list, _, attributes in test_loader:
        # Move data to device
        x_list = [x.to(device) for x in x_list]

        # Get latent representation (mu)
        mu, _ = model.encode(x_list)

        # Store latent vectors and attributes
        latent_vectors.append(mu.cpu().numpy())
        all_attributes.append(attributes.cpu().numpy())

# Concatenate batches
latent_vectors = np.concatenate(latent_vectors, axis=0)
all_attributes = np.concatenate(all_attributes, axis=0)

# Calculate correlations between latent dimensions and attributes
corr_matrix = np.zeros((model.latent_dim, all_attributes.shape[1]))

for i in range(model.latent_dim):
    for j in range(all_attributes.shape[1]):
        corr = np.corrcoef(latent_vectors[:, i], all_attributes[:, j])[0, 1]
        corr_matrix[i, j] = corr

# Plot correlation heatmap
plt.figure(figsize=(10, 8))
sns.heatmap(corr_matrix, cmap='coolwarm', center=0,
            xticklabels=list(model.attribute_dims.keys()),
            yticklabels=[f'z{i+1}' for i in range(model.latent_dim)],
            annot=True, fmt='.2f')

plt.title('Correlation between Latent Dimensions and Clinical Attributes')
plt.xlabel('Clinical Attributes')
plt.ylabel('Latent Dimensions')
plt.tight_layout()
plt.show()

# Print most correlated attributes for each latent dimension
for i in range(model.latent_dim):
    top_attr_idx = np.abs(corr_matrix[i]).argsort()[-3:][::-1]  # Top 3
    top_attrs = [(list(model.attribute_dims.keys())[j], corr_matrix[i, j]) for j in top_a
    print(f"Latent dimension z{i+1} is most correlated with: {top_attrs}")
```

```python
def evaluate_model(model, test_loader, device):
    """
    Evaluate the model on test data

    Args:
        model: Trained model
        test_loader: DataLoader for test data
        device: Device to use

    Returns:
        metrics: Dictionary of test metrics
    """
    # Get test metrics
    test_metrics = model.trainer.validate(test_loader)

    # Print test metrics
    print("Test metrics:")
    for k, v in test_metrics.items():
        print(f"  {k}: {v:.4f}")

    # Calculate predictions for confusion matrix
    model.eval()
    all_preds = []
    all_targets = []

    with torch.no_grad():
        for x_list, y, attributes in test_loader:
            # Move data to device
            x_list = [x.to(device) for x in x_list]

            # Forward pass
            outputs = model(x_list, attributes)
            y_pred = outputs[4]

            # Apply sigmoid and threshold
            y_pred = torch.sigmoid(y_pred).cpu().numpy() > 0.5

            # Store predictions and targets
            all_preds.append(y_pred)
            all_targets.append(y.cpu().numpy())

    # Concatenate batches
```

```python
    all_preds = np.concatenate(all_preds, axis=0).flatten()
    all_targets = np.concatenate(all_targets, axis=0).flatten()

    # Plot confusion matrix
    cm = confusion_matrix(all_targets, all_preds)
    plt.figure(figsize=(8, 6))
    sns.heatmap(cm, annot=True, fmt='d', cmap='Blues',
                xticklabels=['No Complication', 'Complication'],
                yticklabels=['No Complication', 'Complication'])

    plt.title('Confusion Matrix')
    plt.xlabel('Predicted')
    plt.ylabel('Actual')
    plt.tight_layout()
    plt.show()

    return test_metrics
```

```python
# Set up TensorBoard
from torch.utils.tensorboard import SummaryWriter
import datetime

def run_experiment(config=None):
    """
    Run a complete training experiment

    Args:
        config: Dictionary of configuration parameters

    Returns:
        model: Trained model
        history: Training history
    """
    if config is None:
        config = {
            # Model parameters
            'latent_dim': 32,
            'embed_dim': 16,
            'hidden_dim': 64,
            'medical_safety': True,

            # Training parameters
```

```python
        'batch_size': 32,
        'lr': 1e-3,
        'weight_decay': 1e-5,
        'n_epochs': 100,
        'early_stopping_patience': 10,

        # Loss weights
        'beta': 1.0,    # KL weight
        'gamma': 0.1,   # Attribute regularization weight
        'delta': 0.1,   # Medical safety weight
        'lambda_reg': 0.5,  # Group sparsity weight
    }

# Create output directory
timestamp = datetime.datetime.now().strftime("%Y%m%d-%H%M%S")
output_dir = f"./runs/{timestamp}"
os.makedirs(output_dir, exist_ok=True)

# Save configuration
with open(os.path.join(output_dir, 'config.json'), 'w') as f:
    json.dump(config, f, indent=4)

# Create TensorBoard writer
writer = SummaryWriter(output_dir)

# Create TensorBoard callback
tb_callback = TensorboardCallback(writer)

# Load data
print("Loading data...")
X_timepoints, y, attributes = load_mi_data()
train_loader, val_loader, test_loader = create_data_loaders(
    X_timepoints, y, attributes,
    batch_size=config['batch_size']
)

# Get input dimensions and timepoint names
input_dims = [X.shape[1] for X in X_timepoints.values()]
timepoint_names = list(X_timepoints.keys())
attribute_dims = {attr: i for i, attr in enumerate(attributes.columns)}

print(f"Input dimensions: {input_dims}")
```

```
print(f"Timepoint names: {timepoint_names}")
print(f"Attribute dimensions: {attribute_dims}")

# Initialize model
print("Initializing model...")
model = GroupInterpretableVAE(
    input_dims=input_dims,
    timepoint_names=timepoint_names,
    latent_dim=config['latent_dim'],
    embed_dim=config['embed_dim'],
    hidden_dim=config['hidden_dim'],
    attribute_dims=attribute_dims,
    medical_safety=config['medical_safety']
)

# Initialize trainer
trainer = GroupInterpretableVAETrainer(
    model=model,
    train_loader=train_loader,
    val_loader=val_loader,
    device=device,
    lr=config['lr'],
    weight_decay=config['weight_decay'],
    beta=config['beta'],
    gamma=config['gamma'],
    delta=config['delta'],
    lambda_reg=config['lambda_reg'],
    callbacks=[tb_callback]
)

# Train model
print("Training model...")
history, model = trainer.train(
    n_epochs=config['n_epochs'],
    early_stopping_patience=config['early_stopping_patience'],
    checkpoint_dir=os.path.join(output_dir, 'checkpoints')
)

# Attach trainer to model for later evaluation
model.trainer = trainer

# Save final model
```

```
    torch.save({
        'model_state_dict': model.state_dict(),
        'model_config': {
            'input_dims': input_dims,
            'timepoint_names': timepoint_names,
            'latent_dim': config['latent_dim'],
            'embed_dim': config['embed_dim'],
            'hidden_dim': config['hidden_dim'],
            'attribute_dims': attribute_dims,
            'medical_safety': config['medical_safety']
        }
    }, os.path.join(output_dir, 'final_model.pt'))

    # Plot training history
    plot_training_history(history)

    # Visualize latent space
    visualize_latent_space(model, test_loader, device)

    # Visualize group sparsity
    visualize_group_sparsity(model)

    # Visualize attribute regularization
    visualize_attribute_regularization(model, test_loader, device)

    # Evaluate model on test data
    test_metrics = evaluate_model(model, test_loader, device)

    # Save test metrics
    with open(os.path.join(output_dir, 'test_metrics.json'), 'w') as f:
        # Convert values to float for JSON serialization
        test_metrics_json = {k: float(v) for k, v in test_metrics.items()}
        json.dump(test_metrics_json, f, indent=4)

    print(f"Experiment complete. Results saved to {output_dir}")
    print(f"View TensorBoard with: tensorboard --logdir={output_dir}")

    return model, history

# Run the experiment
model, history = run_experiment()
```

```
Loading data...
Loading MI Complications dataset from UCI repository...
Dataset shape: (1700, 111)
Number of samples: 1700
Number of complications: 12
Positive samples (with complications): 1037 (61.00%)
Timepoint admission: 3 features
Timepoint 24h: 0 features
Timepoint 48h: 0 features
Timepoint 72h: 0 features
Selected 6 clinical attributes: ['AGE', 'S_AD_ORIT', 'D_AD_ORIT', 'K_BLOOD', 'L_BLOOD', 'TIM
Timepoint admission: 2.63% missing values
Data preprocessing completed successfully.
Creating train/val/test splits...
Train set: 1190 samples (61.01% positive)
Validation set: 340 samples (60.88% positive)
Test set: 170 samples (61.18% positive)
Data loaders created successfully.
Input dimensions: [3]
Timepoint names: ['admission']
Attribute dimensions: {'AGE': 0, 'S_AD_ORIT': 1, 'D_AD_ORIT': 2, 'K_BLOOD': 3, 'L_BLOOD': 4,
Initializing model...
Training model...
Starting training for 100 epochs with early stopping patience 10

Epoch 1 [Train]:   0%|          | 0/38 [00:00<?, ?it/s]

Validation:   0%|          | 0/11 [00:00<?, ?it/s]

Epoch 1/100 - Train Loss: 1.6367, Val Loss: 1.6965, Train AUROC: 0.5211, Val AUROC: 0.6186
Saved best model at epoch 1 with val_loss: 1.6965

Epoch 2 [Train]:   0%|          | 0/38 [00:00<?, ?it/s]

Validation:   0%|          | 0/11 [00:00<?, ?it/s]

Epoch 2/100 - Train Loss: 1.2683, Val Loss: 1.2480, Train AUROC: 0.5875, Val AUROC: 0.6445
Saved best model at epoch 2 with val_loss: 1.2480

Epoch 3 [Train]:   0%|          | 0/38 [00:00<?, ?it/s]
```

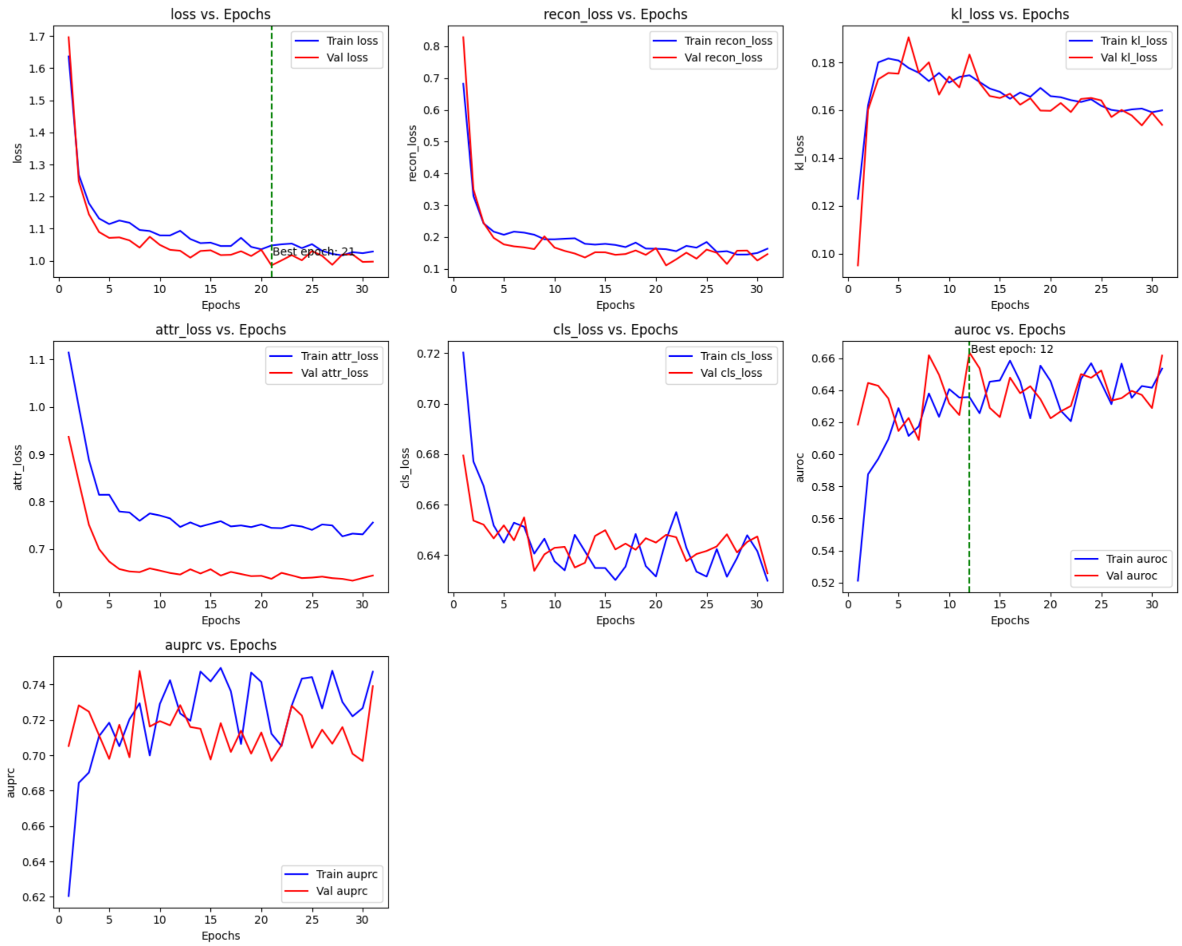
```
Validation:   0%|          | 0/11 [00:00<?, ?it/s]

Epoch 3/100 - Train Loss: 1.1792, Val Loss: 1.1448, Train AUROC: 0.5971, Val AUROC: 0.6428
Saved best model at epoch 3 with val_loss: 1.1448

Epoch 4 [Train]:   0%|          | 0/38 [00:00<?, ?it/s]

Validation:   0%|          | 0/11 [00:00<?, ?it/s]

Epoch 4/100 - Train Loss: 1.1318, Val Loss: 1.0896, Train AUROC: 0.6094, Val AUROC: 0.6348
Saved best model at epoch 4 with val_loss: 1.0896

Epoch 5 [Train]:   0%|          | 0/38 [00:00<?, ?it/s]

Validation:   0%|          | 0/11 [00:00<?, ?it/s]

Epoch 5/100 - Train Loss: 1.1144, Val Loss: 1.0714, Train AUROC: 0.6288, Val AUROC: 0.6145
Saved best model at epoch 5 with val_loss: 1.0714

Epoch 6 [Train]:   0%|          | 0/38 [00:00<?, ?it/s]

Validation:   0%|          | 0/11 [00:00<?, ?it/s]

Epoch 6/100 - Train Loss: 1.1255, Val Loss: 1.0729, Train AUROC: 0.6115, Val AUROC: 0.6226

Epoch 7 [Train]:   0%|          | 0/38 [00:00<?, ?it/s]

Validation:   0%|          | 0/11 [00:00<?, ?it/s]

Epoch 7/100 - Train Loss: 1.1185, Val Loss: 1.0636, Train AUROC: 0.6174, Val AUROC: 0.6089
Saved best model at epoch 7 with val_loss: 1.0636

Epoch 8 [Train]:   0%|          | 0/38 [00:00<?, ?it/s]

Validation:   0%|          | 0/11 [00:00<?, ?it/s]

Epoch 8/100 - Train Loss: 1.0961, Val Loss: 1.0410, Train AUROC: 0.6380, Val AUROC: 0.6618
Saved best model at epoch 8 with val_loss: 1.0410
```

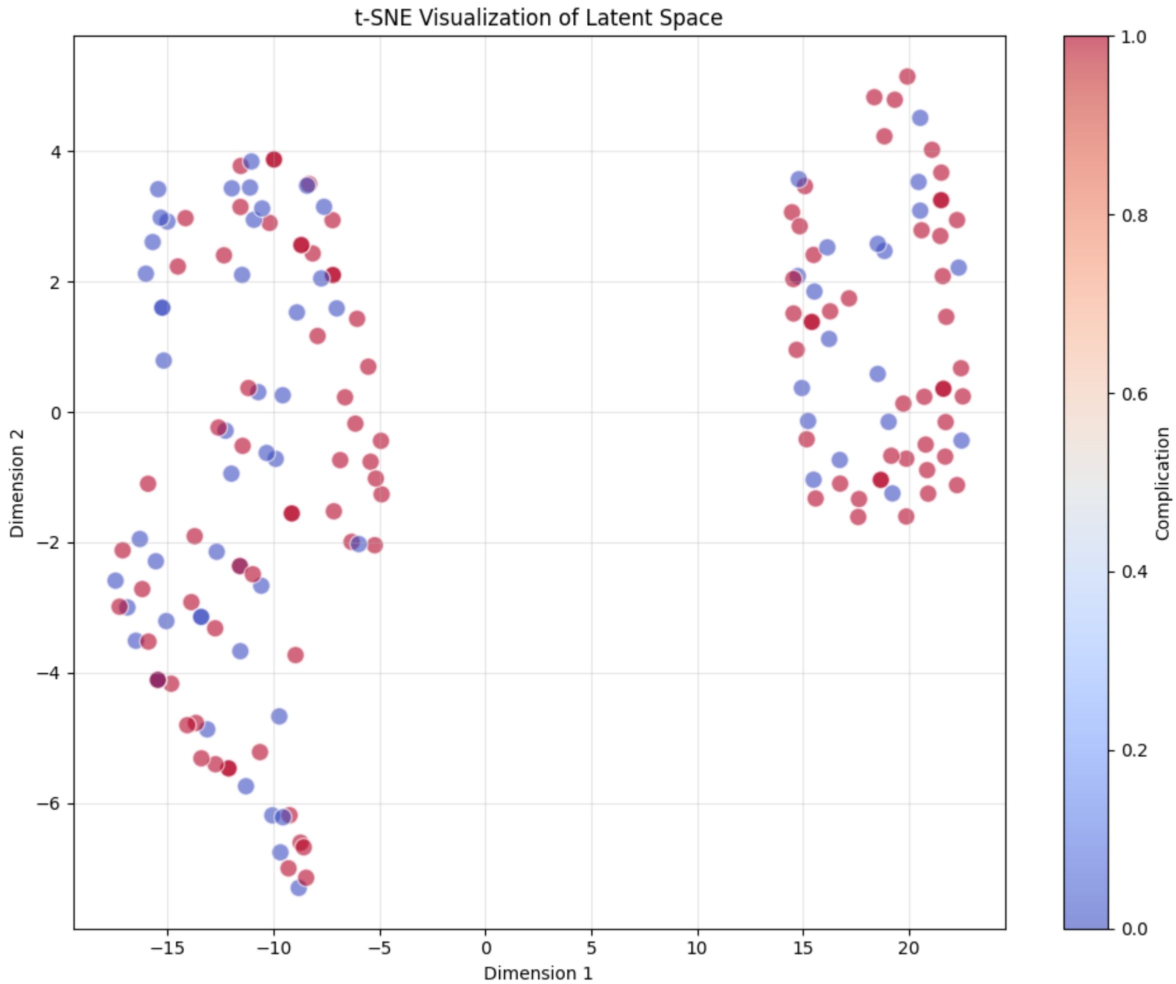
```
Epoch 9 [Train]:   0%|          | 0/38 [00:00<?, ?it/s]

Validation:   0%|          | 0/11 [00:00<?, ?it/s]

Epoch 9/100 - Train Loss: 1.0927, Val Loss: 1.0749, Train AUROC: 0.6234, Val AUROC: 0.6496

Epoch 10 [Train]:   0%|          | 0/38 [00:00<?, ?it/s]

Validation:   0%|          | 0/11 [00:00<?, ?it/s]

Epoch 10/100 - Train Loss: 1.0792, Val Loss: 1.0495, Train AUROC: 0.6407, Val AUROC: 0.6318

Epoch 11 [Train]:   0%|          | 0/38 [00:00<?, ?it/s]

Validation:   0%|          | 0/11 [00:00<?, ?it/s]

Epoch 11/100 - Train Loss: 1.0790, Val Loss: 1.0342, Train AUROC: 0.6354, Val AUROC: 0.6245
Saved best model at epoch 11 with val_loss: 1.0342

Epoch 12 [Train]:   0%|          | 0/38 [00:00<?, ?it/s]

Validation:   0%|          | 0/11 [00:00<?, ?it/s]

Epoch 12/100 - Train Loss: 1.0934, Val Loss: 1.0312, Train AUROC: 0.6357, Val AUROC: 0.6635
Saved best model at epoch 12 with val_loss: 1.0312

Epoch 13 [Train]:   0%|          | 0/38 [00:00<?, ?it/s]

Validation:   0%|          | 0/11 [00:00<?, ?it/s]

Epoch 13/100 - Train Loss: 1.0678, Val Loss: 1.0098, Train AUROC: 0.6256, Val AUROC: 0.6536
Saved best model at epoch 13 with val_loss: 1.0098

Epoch 14 [Train]:   0%|          | 0/38 [00:00<?, ?it/s]

Validation:   0%|          | 0/11 [00:00<?, ?it/s]
```

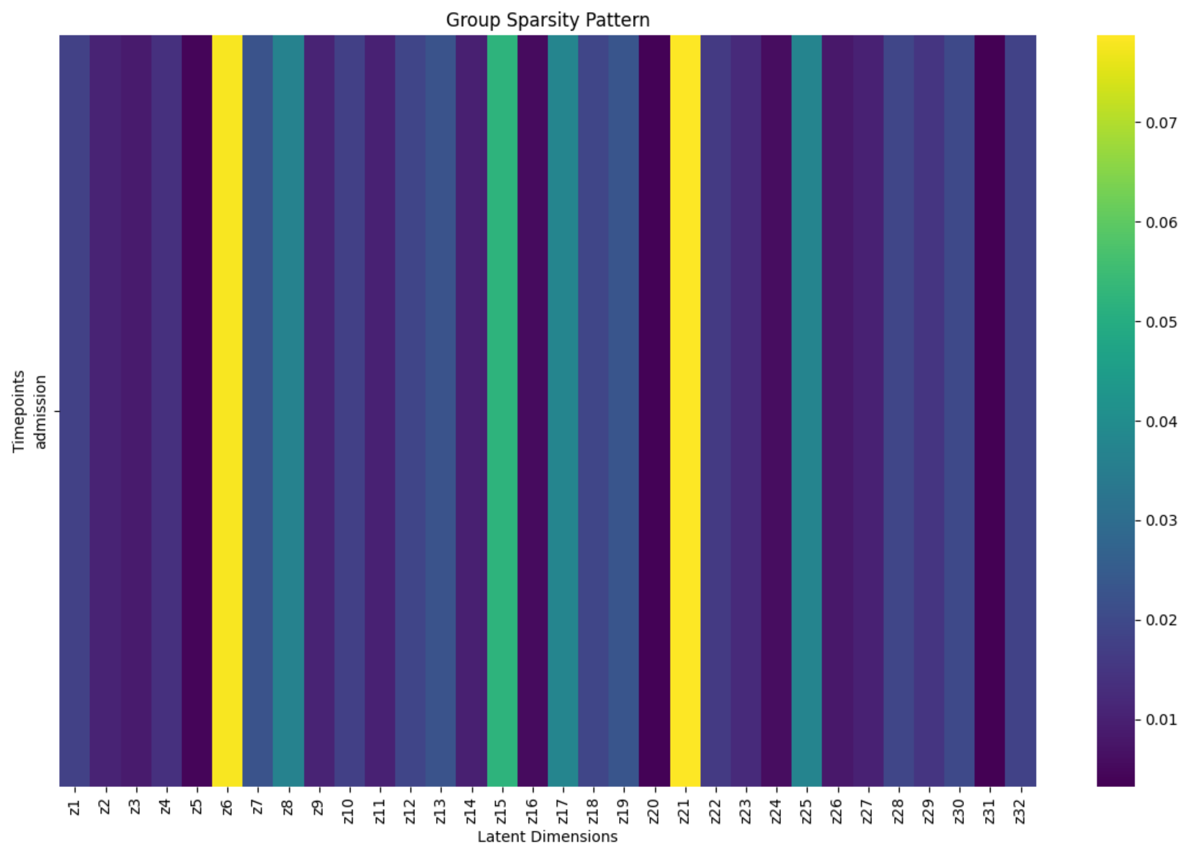
```
Epoch 14/100 - Train Loss: 1.0550, Val Loss: 1.0305, Train AUROC: 0.6453, Val AUROC: 0.6290

Epoch 15 [Train]:   0%|          | 0/38 [00:00<?, ?it/s]

Validation:   0%|          | 0/11 [00:00<?, ?it/s]

Epoch 15/100 - Train Loss: 1.0565, Val Loss: 1.0327, Train AUROC: 0.6461, Val AUROC: 0.6232

Epoch 16 [Train]:   0%|          | 0/38 [00:00<?, ?it/s]

Validation:   0%|          | 0/11 [00:00<?, ?it/s]

Epoch 16/100 - Train Loss: 1.0460, Val Loss: 1.0177, Train AUROC: 0.6584, Val AUROC: 0.6479

Epoch 17 [Train]:   0%|          | 0/38 [00:00<?, ?it/s]

Validation:   0%|          | 0/11 [00:00<?, ?it/s]

Epoch 17/100 - Train Loss: 1.0461, Val Loss: 1.0187, Train AUROC: 0.6455, Val AUROC: 0.6381

Epoch 18 [Train]:   0%|          | 0/38 [00:00<?, ?it/s]

Validation:   0%|          | 0/11 [00:00<?, ?it/s]

Epoch 18/100 - Train Loss: 1.0714, Val Loss: 1.0298, Train AUROC: 0.6224, Val AUROC: 0.6425

Epoch 19 [Train]:   0%|          | 0/38 [00:00<?, ?it/s]

Validation:   0%|          | 0/11 [00:00<?, ?it/s]

Epoch 19/100 - Train Loss: 1.0434, Val Loss: 1.0149, Train AUROC: 0.6553, Val AUROC: 0.6344

Epoch 20 [Train]:   0%|          | 0/38 [00:00<?, ?it/s]

Validation:   0%|          | 0/11 [00:00<?, ?it/s]

Epoch 20/100 - Train Loss: 1.0358, Val Loss: 1.0342, Train AUROC: 0.6456, Val AUROC: 0.6225
```

```
Epoch 21 [Train]:   0%|          | 0/38 [00:00<?, ?it/s]

Validation:   0%|          | 0/11 [00:00<?, ?it/s]

Epoch 21/100 - Train Loss: 1.0477, Val Loss: 0.9856, Train AUROC: 0.6273, Val AUROC: 0.6268
Saved best model at epoch 21 with val_loss: 0.9856

Epoch 22 [Train]:   0%|          | 0/38 [00:00<?, ?it/s]

Validation:   0%|          | 0/11 [00:00<?, ?it/s]

Epoch 22/100 - Train Loss: 1.0513, Val Loss: 1.0012, Train AUROC: 0.6206, Val AUROC: 0.6301

Epoch 23 [Train]:   0%|          | 0/38 [00:00<?, ?it/s]

Validation:   0%|          | 0/11 [00:00<?, ?it/s]

Epoch 23/100 - Train Loss: 1.0536, Val Loss: 1.0176, Train AUROC: 0.6470, Val AUROC: 0.6500

Epoch 24 [Train]:   0%|          | 0/38 [00:00<?, ?it/s]

Validation:   0%|          | 0/11 [00:00<?, ?it/s]

Epoch 24/100 - Train Loss: 1.0395, Val Loss: 1.0015, Train AUROC: 0.6568, Val AUROC: 0.6477

Epoch 25 [Train]:   0%|          | 0/38 [00:00<?, ?it/s]

Validation:   0%|          | 0/11 [00:00<?, ?it/s]

Epoch 25/100 - Train Loss: 1.0517, Val Loss: 1.0303, Train AUROC: 0.6445, Val AUROC: 0.6523

Epoch 26 [Train]:   0%|          | 0/38 [00:00<?, ?it/s]

Validation:   0%|          | 0/11 [00:00<?, ?it/s]

Epoch 26/100 - Train Loss: 1.0310, Val Loss: 1.0154, Train AUROC: 0.6313, Val AUROC: 0.6335
```

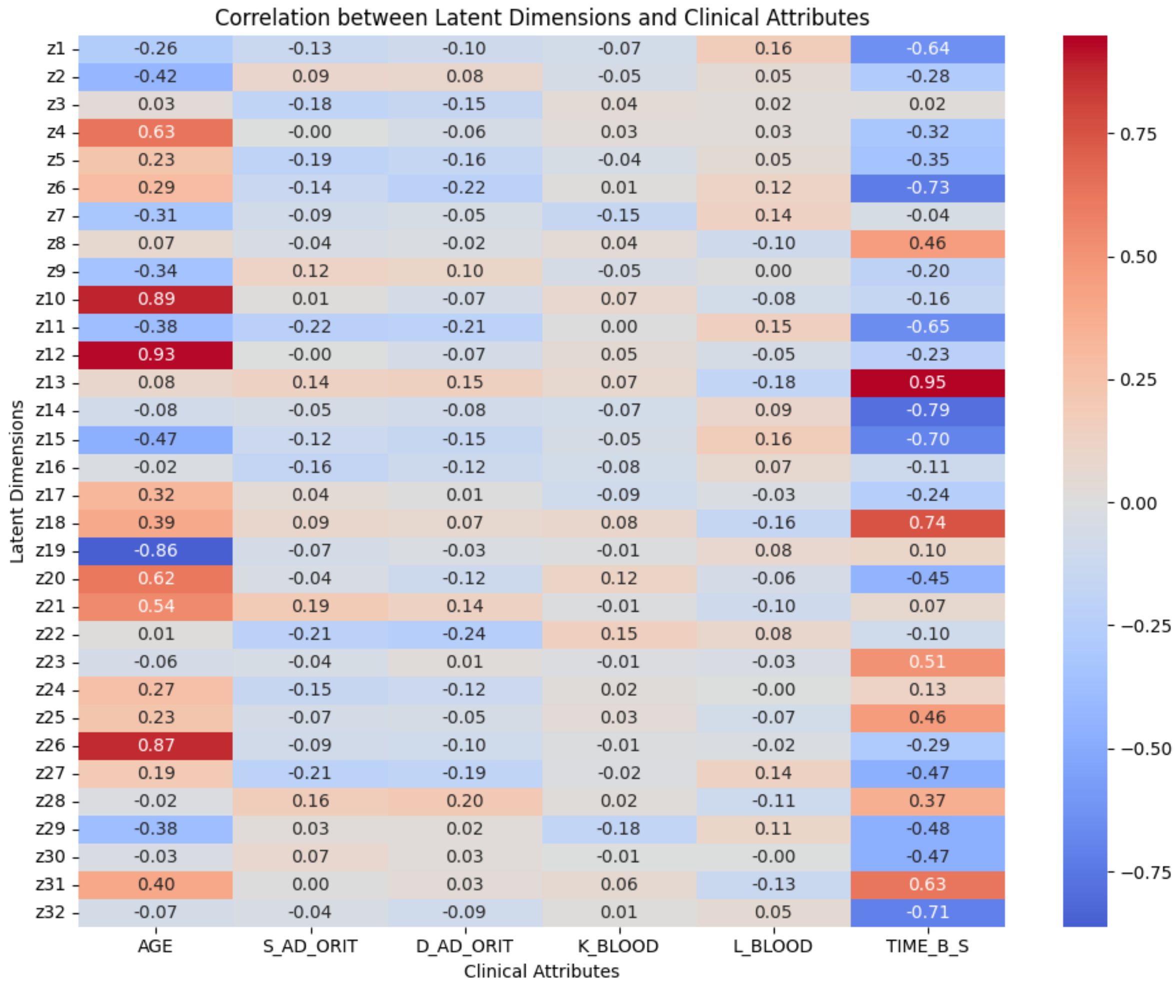
```
Epoch 27 [Train]:   0%|          | 0/38 [00:00<?, ?it/s]

Validation:   0%|          | 0/11 [00:00<?, ?it/s]

Epoch 27/100 - Train Loss: 1.0215, Val Loss: 0.9876, Train AUROC: 0.6566, Val AUROC: 0.6350

Epoch 28 [Train]:   0%|          | 0/38 [00:00<?, ?it/s]

Validation:   0%|          | 0/11 [00:00<?, ?it/s]

Epoch 28/100 - Train Loss: 1.0168, Val Loss: 1.0195, Train AUROC: 0.6352, Val AUROC: 0.6396

Epoch 29 [Train]:   0%|          | 0/38 [00:00<?, ?it/s]

Validation:   0%|          | 0/11 [00:00<?, ?it/s]

Epoch 29/100 - Train Loss: 1.0269, Val Loss: 1.0197, Train AUROC: 0.6426, Val AUROC: 0.6370

Epoch 30 [Train]:   0%|          | 0/38 [00:00<?, ?it/s]

Validation:   0%|          | 0/11 [00:00<?, ?it/s]

Epoch 30/100 - Train Loss: 1.0237, Val Loss: 0.9964, Train AUROC: 0.6415, Val AUROC: 0.6289

Epoch 31 [Train]:   0%|          | 0/38 [00:00<?, ?it/s]

Validation:   0%|          | 0/11 [00:00<?, ?it/s]

Epoch 31/100 - Train Loss: 1.0288, Val Loss: 0.9974, Train AUROC: 0.6535, Val AUROC: 0.6616
Early stopping triggered after 31 epochs
```


loss vs. Epochs
Train loss
Val loss
Best epoch: 21
loss
Epochs
recon_loss vs. Epochs
Train recon_loss
Val recon_loss
recon_loss
Epochs
kl_loss vs. Epochs
Train kl_loss
Val kl_loss
kl_loss
Epochs
attr_loss vs. Epochs
Train attr_loss
Val attr_loss
attr_loss
Epochs
cls_loss vs. Epochs
Train cls_loss
Val cls_loss
cls_loss
Epochs
auroc vs. Epochs
Best epoch: 12
Train auroc
Val auroc
auroc
Epochs
auprc vs. Epochs
Train auprc
Val auprc
auprc
Epochs


t-SNE Visualization of Latent Space
Dimension 1
Dimension 2
−15
−10
−5
0
5
10
15
20
4
2
0
−2
−4
−6
Complication
1.0
0.8
0.6
0.4
0.2
0.0

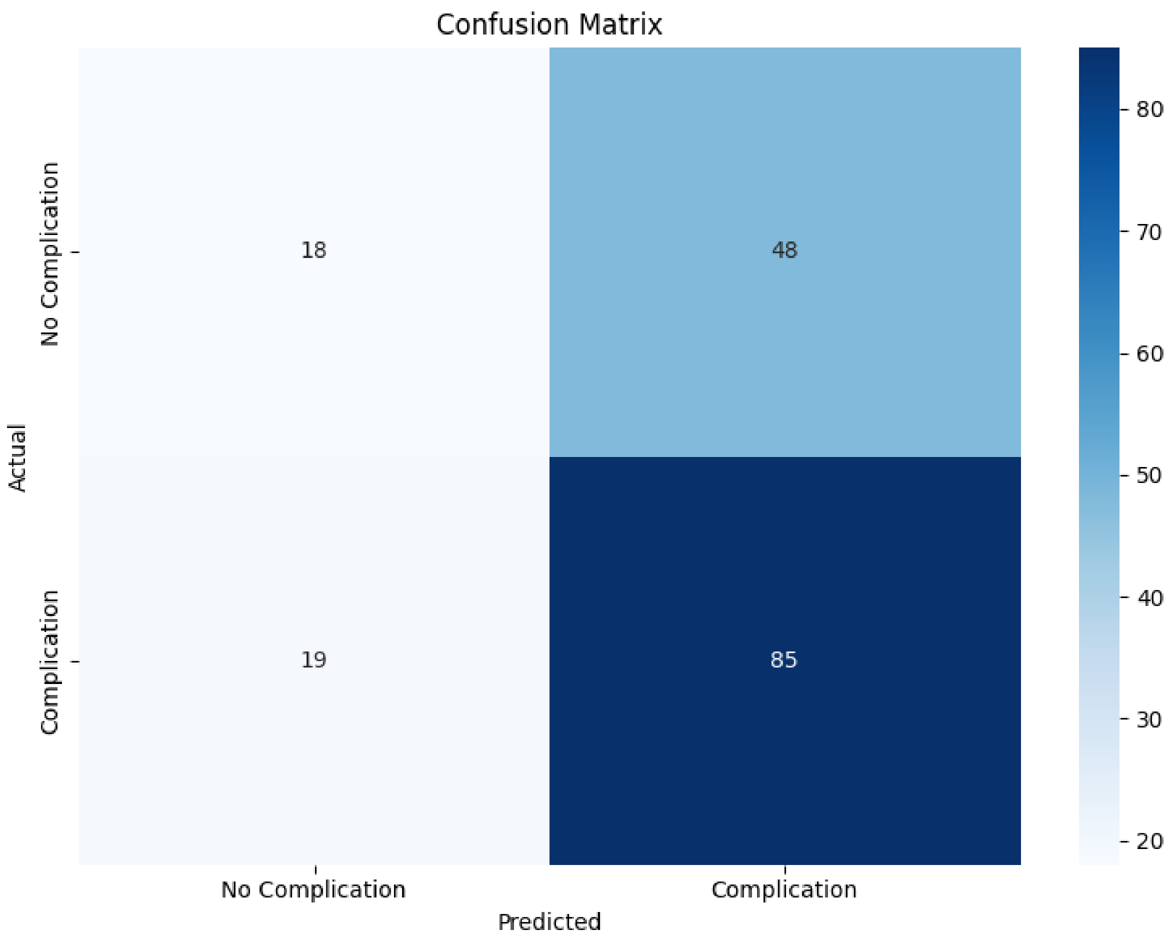


Timepoint admission is influenced by latent dimensions: []




```
Latent dimension z1 is most correlated with: [('TIME_B_S', np.float64(-0.6377436265755303)),
Latent dimension z2 is most correlated with: [('AGE', np.float64(-0.41800312911144777)), ('T
Latent dimension z3 is most correlated with: [('S_AD_ORIT', np.float64(-0.1842425731977365))
Latent dimension z4 is most correlated with: [('AGE', np.float64(0.6342007109107097)), ('TIM
Latent dimension z5 is most correlated with: [('TIME_B_S', np.float64(-0.34579389919543563))
Latent dimension z6 is most correlated with: [('TIME_B_S', np.float64(-0.7280939836684573)),
Latent dimension z7 is most correlated with: [('AGE', np.float64(-0.313516619442179)), ('K_B
Latent dimension z8 is most correlated with: [('TIME_B_S', np.float64(0.45559995667911973)),
Latent dimension z9 is most correlated with: [('AGE', np.float64(-0.3431252115532879)), ('TI
Latent dimension z10 is most correlated with: [('AGE', np.float64(0.8897627722811079)), ('TI
Latent dimension z11 is most correlated with: [('TIME_B_S', np.float64(-0.6517921717200551))
Latent dimension z12 is most correlated with: [('AGE', np.float64(0.9294212512777801)), ('TI
Latent dimension z13 is most correlated with: [('TIME_B_S', np.float64(0.9474185916893575)),
Latent dimension z14 is most correlated with: [('TIME_B_S', np.float64(-0.7869936919339381))
```

```
Latent dimension z15 is most correlated with: [('TIME_B_S', np.float64(-0.6971735505807037))
Latent dimension z16 is most correlated with: [('S_AD_ORIT', np.float64(-0.16445866893025324
Latent dimension z17 is most correlated with: [('AGE', np.float64(0.3243954744348347)), ('TI
Latent dimension z18 is most correlated with: [('TIME_B_S', np.float64(0.7449000791157308)),
Latent dimension z19 is most correlated with: [('AGE', np.float64(-0.8620416975866418)), ('T
Latent dimension z20 is most correlated with: [('AGE', np.float64(0.6177065356762959)), ('TI
Latent dimension z21 is most correlated with: [('AGE', np.float64(0.5387503236709416)), ('S_
Latent dimension z22 is most correlated with: [('D_AD_ORIT', np.float64(-0.24146180427697553
Latent dimension z23 is most correlated with: [('TIME_B_S', np.float64(0.5080572993263404)),
Latent dimension z24 is most correlated with: [('AGE', np.float64(0.26538603210319356)), ('S
Latent dimension z25 is most correlated with: [('TIME_B_S', np.float64(0.4620892951812275)),
Latent dimension z26 is most correlated with: [('AGE', np.float64(0.8740096872569565)), ('TI
Latent dimension z27 is most correlated with: [('TIME_B_S', np.float64(-0.4716705271016905))
Latent dimension z28 is most correlated with: [('TIME_B_S', np.float64(0.36638965051109923))
Latent dimension z29 is most correlated with: [('TIME_B_S', np.float64(-0.47575436629615836)
Latent dimension z30 is most correlated with: [('TIME_B_S', np.float64(-0.4748258954726793))
Latent dimension z31 is most correlated with: [('TIME_B_S', np.float64(0.6256528170199492)),
Latent dimension z32 is most correlated with: [('TIME_B_S', np.float64(-0.7072562966673279))

Validation:   0%|          | 0/6 [00:00<?, ?it/s]

Test metrics:
  loss: 1.0215
  recon_loss: 0.1466
  kl_loss: 0.1715
  attr_loss: 0.7239
  cls_loss: 0.6310
  auroc: 0.6719
  auprc: 0.7851
```




```
Experiment complete. Results saved to ./runs/20250424-025550
View TensorBoard with: tensorboard --logdir=./runs/20250424-025550
```