[CLS] TSK_pytorch

October 3, 2025

[1]:
```
import numpy as np
from sklearn import datasets
from sklearn.preprocessing import StandardScaler
from sklearn.model_selection import train_test_split
from sklearn.metrics import␣
↪mean_squared_error,accuracy_score,classification_report,confusion_matrix,ConfusionMatrixDis
import skfuzzy as fuzz
import matplotlib.pyplot as plt
import torch
import torch.nn as nn
import torch.optim as optim
import pandas

import copy
import itertools
```

[2]:
```
# CHOOSE DATASET

# Binary classification dataset
data = datasets.fetch_openml(name="diabetes",version=1, as_frame=True)

X = data.data.values
y = data.target.values
X.shape

# Keep as DataFrame for named-column ops
df = data.data.copy()
y = np.where(data.target.values == "tested_positive", 1, 0).astype(np.float32)

# indices of features with invalid zeros
invalid_idx = [1, 2, 3, 4, 5, 7]

# count zeros per feature
zero_counts = (X[:, invalid_idx] == 0).sum(axis=0)
rows_with_zero = (X[:, invalid_idx] == 0).any(axis=1).sum()

print("Zeros per feature:\n", zero_counts)
```

```
print(f"Rows with  1 zero: {rows_with_zero} / {len(df)}")

(len(X), zero_counts, rows_with_zero)

# Drop columns 3 and 4 (0-based indexing)
X = np.delete(X, [3, 4], axis=1)

# Keep only rows where Glucose, BloodPressure, BMI are non-zero
mask = (X[:, [1, 2, 3, 4]] != 0).all(axis=1)
X = X[mask]
y = y[mask]
```

```
Zeros per feature:
 [  5  35 227 374  11   0]
Rows with  1 zero: 376 / 768
```

[3]:
```
#train test spliting
test_size=0.2
Xtr, Xte, ytr, yte = train_test_split(X, y, test_size=test_size,
 ↪random_state=42)
```

[4]:
```
# Standardize features
scaler=StandardScaler()
Xtr= scaler.fit_transform(Xtr)
Xte= scaler.transform(Xte)
```

[5]:
```
 # Number of clusters
n_clusters = 2
m=1.5

# Concatenate target for clustering
Xexp=np.concatenate([Xtr, ytr.reshape(-1, 1)], axis=1)
#Xexp=Xtr

# Transpose data for skfuzzy (expects features x samples)
Xexp_T = Xexp.T

# Fuzzy C-means clustering
centers, u, u0, d, jm, p, fpc = fuzz.cluster.cmeans(
    Xexp_T, n_clusters, m=m, error=0.005, maxiter=1000, init=None,
)
```

[6]:
```
centers.shape
```

[6]:
```
(2, 7)
```

[7]:
```
# Compute sigma (spread) for each cluster
sigmas = []
```

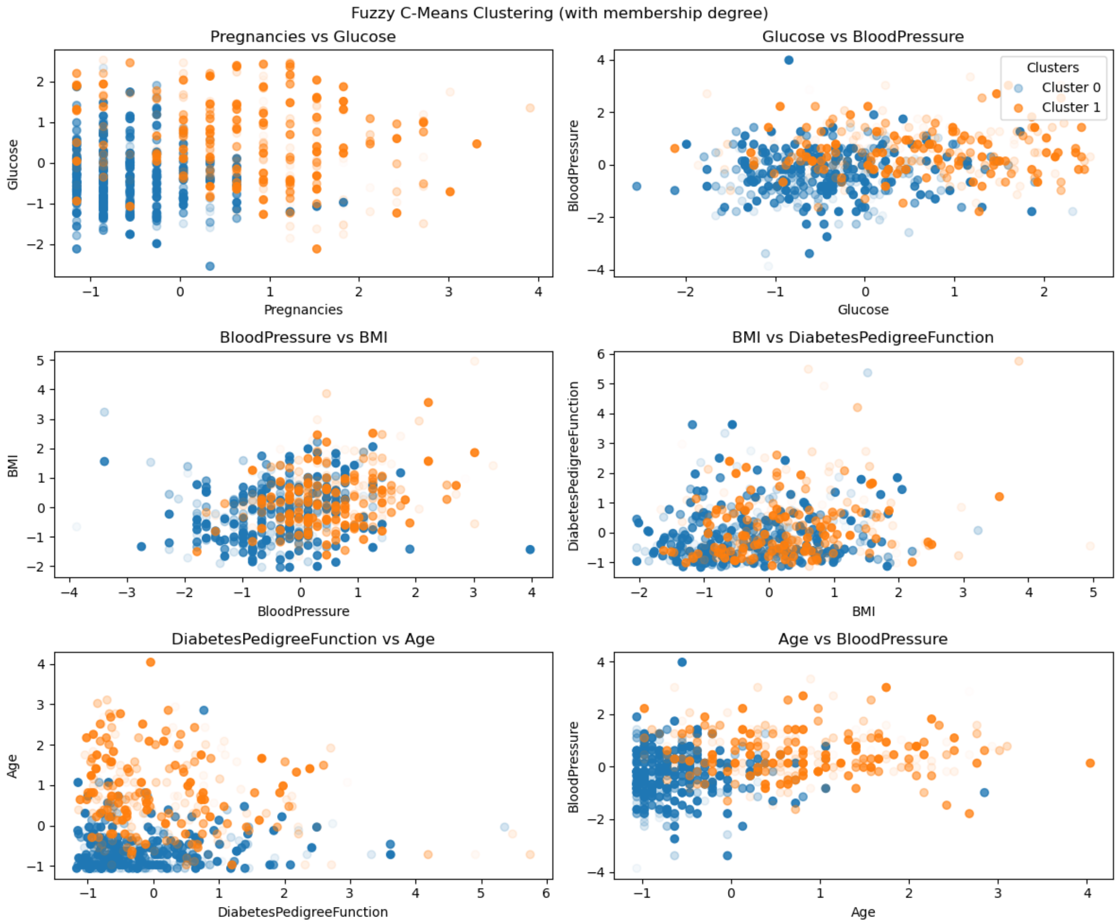
```python
for j in range(n_clusters):
    # membership weights for cluster j, raised to m
    u_j = u[j, :] ** m
    # weighted variance for each feature
    var_j = np.average((Xexp - centers[j])**2, axis=0, weights=u_j)
    sigma_j = np.sqrt(var_j)
    sigmas.append(sigma_j)
sigmas=np.array(sigmas)
```

[8]:

```python
# Hard clustering from fuzzy membership
cluster_labels = np.argmax(u, axis=0)
print("Fuzzy partition coefficient (FPC):", fpc)

feature_names = [
    "Pregnancies", "Glucose", "BloodPressure",
    "BMI", "DiabetesPedigreeFunction", "Age"
]

# Choose 4 feature pairs (indices in Xexp)
pairs = [(0, 1),  # Pregnancies vs Glucose
         (1, 2),  # Glucose vs BloodPressure
         (2, 3),  # BloodPressure vs BMI
         (3, 4),  # BMI vs Pedigree
         (4, 5),  # Pedigree vs Age
         (5, 2)]  # Age vs Glucose

fig, axes = plt.subplots(3, 2, figsize=(12, 10))

for ax, (i, j) in zip(axes.ravel(), pairs):
    # Plot 2 features with fuzzy membership
    for k in range(n_clusters):
        ax.scatter(
            Xexp[cluster_labels == k, i],             # Feature 1
            Xexp[cluster_labels == k, j],             # Feature 2
            alpha=u[k, :],          # transparency ~ membership
            label=f'Cluster {k}'
        )

    ax.set_xlabel(feature_names[i])
    ax.set_ylabel(feature_names[j])
    ax.set_title(f"{feature_names[i]} vs {feature_names[j]}")

fig.suptitle("Fuzzy C-Means Clustering (with membership degree)")
axes[0,1].legend(title="Clusters", loc="upper right")
plt.tight_layout()
plt.show()
```

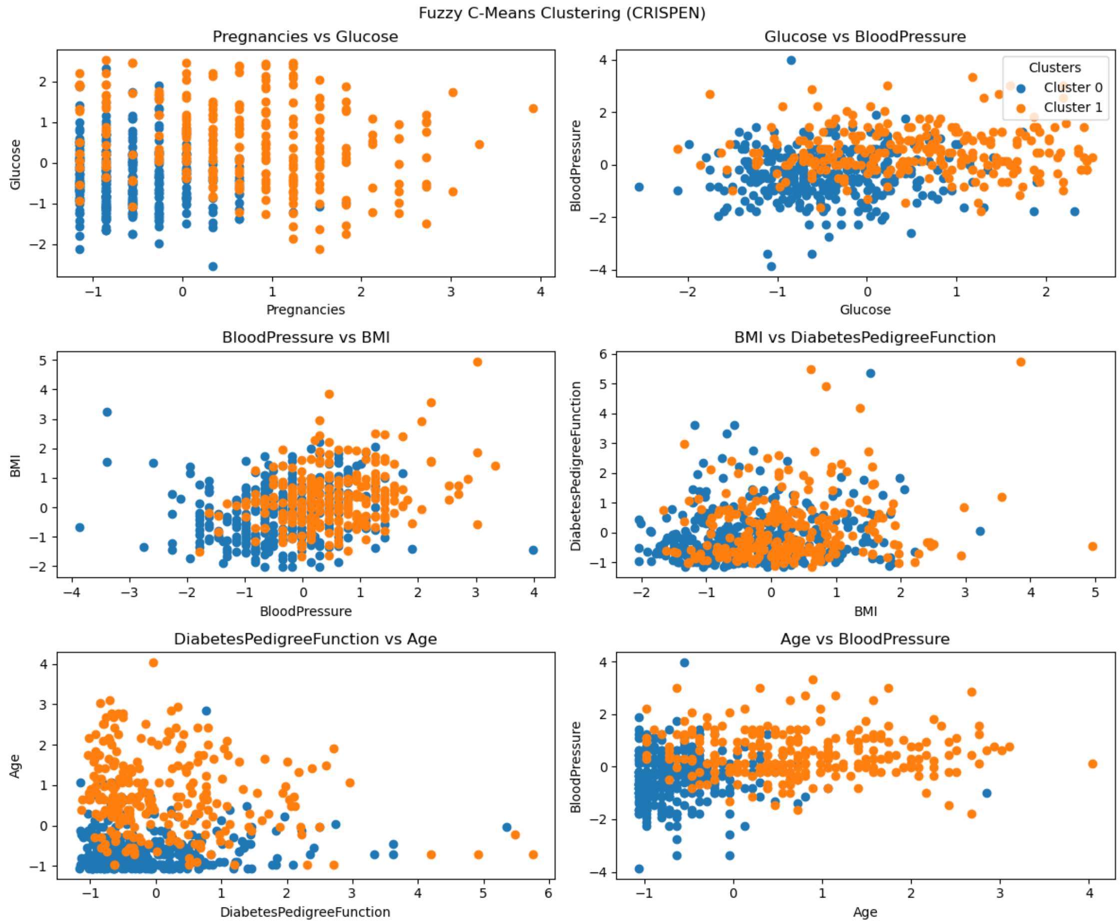
```
fig.savefig("../Plots/Fuzzy C-Means Clustering (with membership degree) CLF.
↪pdf", format="pdf", bbox_inches="tight")
```

```
Fuzzy partition coefficient (FPC): 0.7231777903765536
```



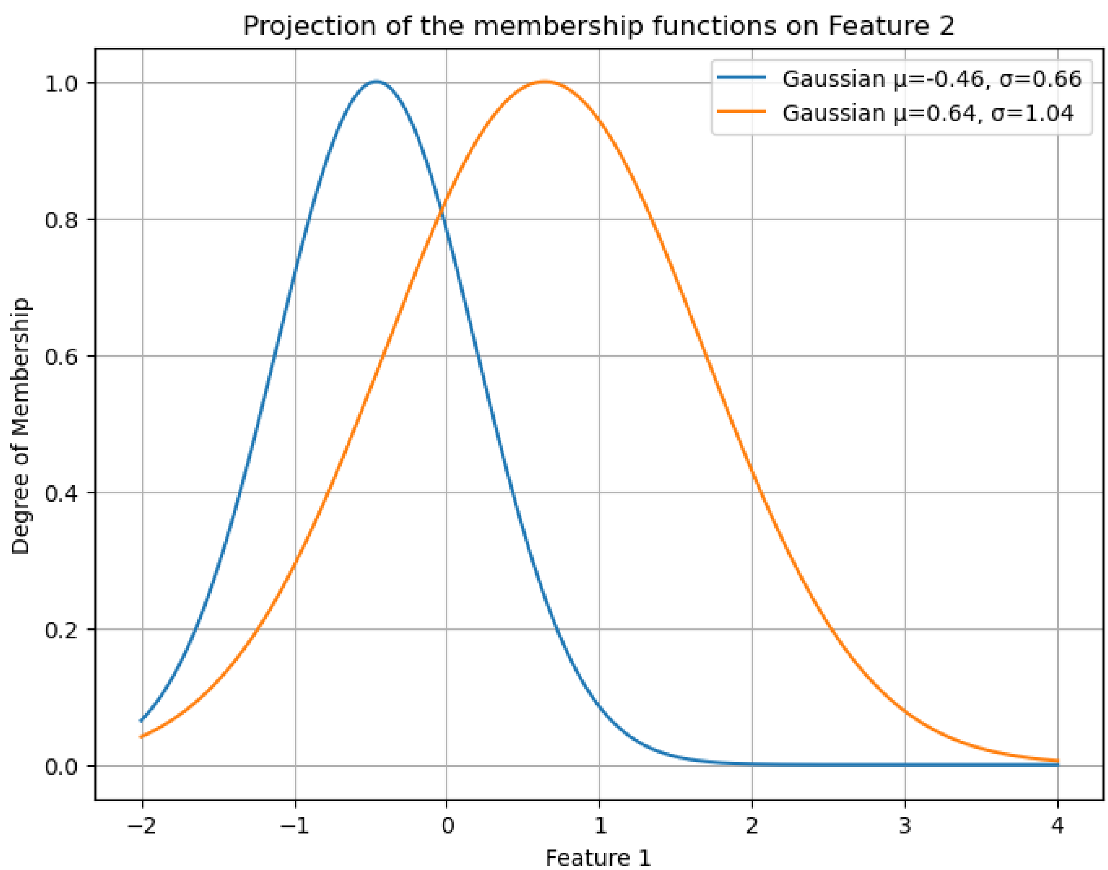
[9]:
```
fig, axes = plt.subplots(3, 2, figsize=(12, 10))

for ax, (i, j) in zip(axes.ravel(), pairs):
    # Plot 2 features with fuzzy membership
    for k in range(n_clusters):
        ax.scatter(
            Xexp[cluster_labels == k, i],
            Xexp[cluster_labels == k, j],
            label=f'Cluster {k}'
        )

    ax.set_xlabel(feature_names[i])
    ax.set_ylabel(feature_names[j])
```

```
    ax.set_title(f"{feature_names[i]} vs {feature_names[j]}")

fig.suptitle("Fuzzy C-Means Clustering (CRISPEN)")
axes[0,1].legend(title="Clusters", loc="upper right")
fig.tight_layout()
fig.show()

fig.savefig("../Plots/Fuzzy C-Means Clustering (CRISPEN) CLF.pdf",␣
 ↪format="pdf", bbox_inches="tight")
```



[10]:
```
# Gaussian formula
def gaussian(x, mu, sigma):
    return np.exp(-0.5 * ((x - mu)/sigma)**2)

lin=np.linspace(-2, 4, 500)
plt.figure(figsize=(8,6))

y_aux=[]
```

```
feature=0
for j in range(n_clusters):
# Compute curves
    y_aux.append(gaussian(lin, centers[j,feature], sigmas[j,feature]))

# Plot
    plt.plot(lin, y_aux[j], label=f"Gaussian  ={np.
 ↪round(centers[j,feature],2)},  ={np.round(sigmas[j,feature],2)}")

plt.title("Projection of the membership functions on Feature 2")
plt.xlabel("Feature 1")
plt.ylabel("Degree of Membership")
plt.legend()
plt.grid(True)
plt.show()
```




```
[11]: # ---------------------------
# Gaussian Membership Function
# ---------------------------
```

```
class GaussianMF(nn.Module):
    def __init__(self, centers, sigmas, agg_prob):
        super().__init__()
        self.centers = nn.Parameter(torch.tensor(centers, dtype=torch.float32))
        self.sigmas = nn.Parameter(torch.tensor(sigmas, dtype=torch.float32))
        self.agg_prob=agg_prob

    def forward(self, x):
        # Expand for broadcasting
        # x: (batch, 1, n_dims), centers: (1, n_rules, n_dims), sigmas: (1,
↪n_rules, n_dims)
        diff = abs((x.unsqueeze(1) - self.centers.unsqueeze(0))/self.sigmas.
↪unsqueeze(0)) #(batch, n_rules, n_dims)

        # Aggregation
        if self.agg_prob:
            dist = torch.norm(diff, dim=-1)  # (batch, n_rules) # probablistic
↪intersection
        else:
            dist = torch.max(diff, dim=-1).values  # (batch, n_rules) # min
↪intersection (min instersection of normal funtion is the same as the max on
↪dist)

        return torch.exp(-0.5 * dist ** 2)


# ---------------------------
# TSK Model
# ---------------------------
class TSK(nn.Module):
    def __init__(self, n_inputs, n_rules, centers, sigmas,agg_prob=False):
        super().__init__()
        self.n_inputs = n_inputs
        self.n_rules = n_rules

        # Antecedents (Gaussian MFs)

        self.mfs=GaussianMF(centers, sigmas,agg_prob)

        # Consequents (linear functions of inputs)
        # Each rule has coeffs for each input + bias
        self.consequents = nn.Parameter(
            torch.randn(n_inputs + 1,n_rules)
        )

    def forward(self, x):
        # x: (batch, n_inputs)
```

```
        batch_size = x.shape[0]

        # Compute membership values for each input feature
        # firing_strengths: (batch, n_rules)
        firing_strengths = self.mfs(x)

        # Normalize memberships
        # norm_fs: (batch, n_rules)
        norm_fs = firing_strengths / (firing_strengths.sum(dim=1, keepdim=True)␣
 ↪+ 1e-9)

        # Consequent output (linear model per rule)
        x_aug = torch.cat([x, torch.ones(batch_size, 1)], dim=1)  # add bias

        rule_outputs = torch.einsum("br,rk->bk", x_aug, self.consequents)  #␣
 ↪(batch, rules)
        # Weighted sum
        output = torch.sum(norm_fs * rule_outputs, dim=1, keepdim=True)

        return output, norm_fs, rule_outputs
```

[12]:

```
# ---------------------------
# Least Squares Solver for Consequents (TSK)
# ---------------------------
def train_ls(model, X, y):
    with torch.no_grad():
        _, norm_fs, _ = model(X)

        # Design matrix for LS: combine normalized firing strengths with input
        X_aug = torch.cat([X, torch.ones(X.shape[0], 1)], dim=1)

        Phi = torch.einsum("br,bi->bri", X_aug, norm_fs).reshape(X.shape[0], -1)

        # Solve LS: consequents = (Phi^T Phi)^-1 Phi^T y

        theta= torch.linalg.lstsq(Phi, y).solution


        model.consequents.data = theta.reshape(model.consequents.shape)
```

[13]:

```
# ---------------------------
# Gradient Descent Training
# ---------------------------
def train_gd(model, X, y, epochs=100, lr=1e-3):
    optimizer = optim.Adam(model.parameters(), lr=lr)
```

```python
    criterion = nn.MSELoss()
    for _ in range(epochs):
        optimizer.zero_grad()
        y_pred, _, _ = model(X)
        loss = criterion(y_pred, y)
        #print(loss)
        loss.backward()
        optimizer.step()
```

[14]:
```python
# ---------------------------
# Hybrid Training (Classic ANFIS)
# ---------------------------
def train_hybrid_anfis(model, X, y, max_iters=10, gd_epochs=20, lr=1e-3):
    train_ls(model, X, y)
    for _ in range(max_iters):
        # Step A: GD on antecedents (freeze consequents)
        model.consequents.requires_grad = False
        train_gd(model, X, y, epochs=gd_epochs, lr=lr)

        # Step B: LS on consequents (freeze antecedents)
        model.consequents.requires_grad = True
        model.mfs.requires_grad = False
        train_ls(model, X, y)

        # Re-enable antecedents
        model.mfs.requires_grad = True
```

[15]:
```python
# ---------------------------
# Alternative Hybrid Training (LS+ gradient descent on all)
# ---------------------------
def train_hybrid(model, X, y, epochs=100, lr=1e-4):
    # Step 1: LS for consequents
    train_ls(model, X, y)
    # Step 2: GD fine-tuning
    train_gd(model, X, y, epochs=epochs, lr=lr)
```

[16]:
```python
# Build model
model = TSK(n_inputs=Xtr.shape[1], n_rules=n_clusters, centers=centers[:,:-1],␣
↪sigmas=sigmas[:,:-1])

Xtr = torch.tensor(Xtr, dtype=torch.float32)
ytr = torch.tensor(ytr, dtype=torch.float32)
Xte = torch.tensor(Xte, dtype=torch.float32)
yte = torch.tensor(yte, dtype=torch.float32)
```

[17]:
```python
param_grid = {
    "max_iters": [3, 5, 7],
```

```
    "gd_epochs": [10, 20, 50],
    "lr": [1e-2, 1e-3, 3e-4]
}

results = []

for max_iters, gd_epochs, lr in itertools.product(
    param_grid["max_iters"],
    param_grid["gd_epochs"],
    param_grid["lr"]
):
    m = copy.deepcopy(model)
    train_hybrid_anfis(m, Xtr, ytr.reshape(-1,1),
                       max_iters=max_iters,
                       gd_epochs=gd_epochs,
                       lr=lr)

    # forward pass
    y_pred, _, _ = m(Xte)

    # compute accuracy
    acc = accuracy_score(
        yte.detach().cpu().numpy(),
        (y_pred.detach().cpu().numpy() > 0.5)
    )

    # save result as dict
    results.append({
        "max_iters": max_iters,
        "gd_epochs": gd_epochs,
        "lr": lr,
        "accuracy": acc
    })

# Convert to DataFrame
df = pandas.DataFrame(results)

# Sort by accuracy (descending)
df = df.sort_values(by="accuracy", ascending=False).reset_index(drop=True)

print(df)
```

```
   max_iters  gd_epochs      lr  accuracy
0          3         10  0.0100  0.820690
1          5         50  0.0010  0.820690
2          3         50  0.0100  0.806897
3          7         20  0.0100  0.806897
4          7         50  0.0010  0.806897
```

5	5	50	0.0100	0.806897
6	3	50	0.0003	0.800000
7	3	10	0.0003	0.800000
8	3	20	0.0003	0.800000
9	5	10	0.0100	0.800000
10	3	10	0.0010	0.800000
11	7	10	0.0003	0.800000
12	7	20	0.0003	0.800000
13	5	10	0.0003	0.800000
14	5	10	0.0010	0.800000
15	5	20	0.0003	0.800000
16	5	20	0.0100	0.800000
17	3	20	0.0010	0.793103
18	3	20	0.0100	0.793103
19	7	10	0.0100	0.793103
20	3	50	0.0010	0.786207
21	5	50	0.0003	0.786207
22	5	20	0.0010	0.786207
23	7	20	0.0010	0.786207
24	7	10	0.0010	0.786207
25	7	50	0.0100	0.786207
26	7	50	0.0003	0.786207

[18]:
```python
# Training with LS:
model_ls = copy.deepcopy(model)
train_ls(model_ls, Xtr, ytr.reshape(-1,1))

# Training with GD:
model_gd = copy.deepcopy(model)
train_gd(model_gd, Xtr, ytr.reshape(-1,1), epochs=100, lr=1e-3)

# Training with Hybrid (Classic ANFIS):
model_h = copy.deepcopy(model)
train_hybrid_anfis(model_h, Xtr, ytr.reshape(-1,1), max_iters=3, gd_epochs=10,␣
  ↪lr=1e-2)

# Training with Alternative Hybrid (LS + GD):
model_ah = copy.deepcopy(model)
train_hybrid(model_ah, Xtr, ytr.reshape(-1,1), epochs=100, lr=1e-4)
```

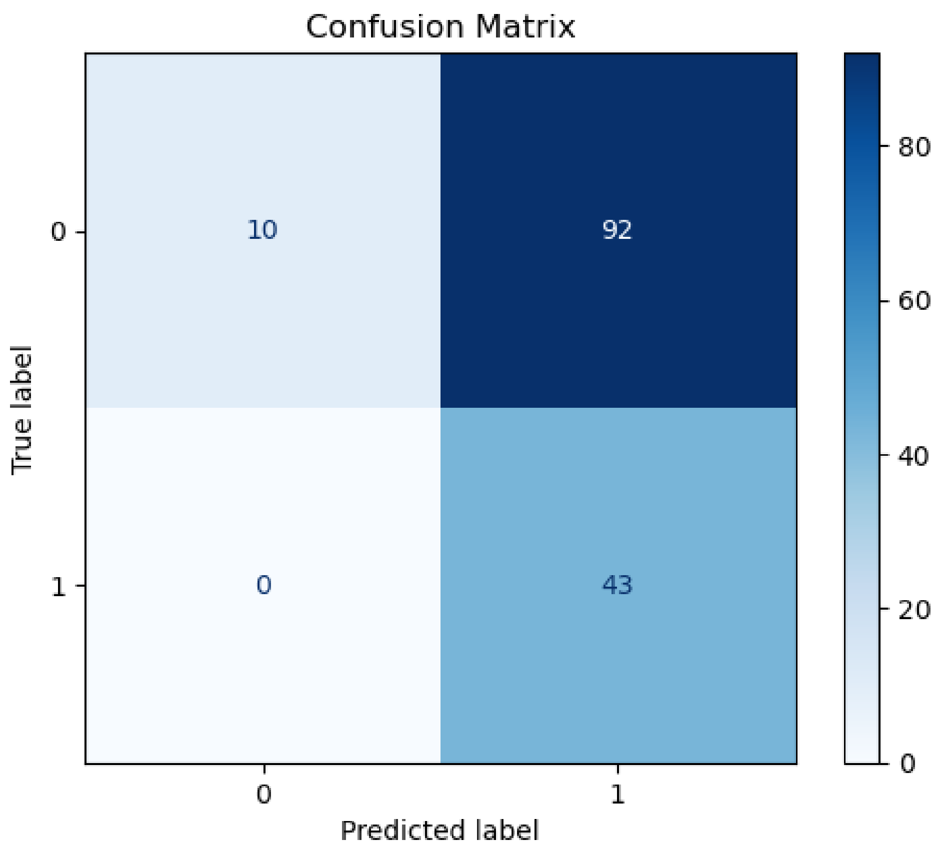
[19]:
```python
y_pred, _, _=model_ls(Xte)
#performance metric for classification
print(f'LS ACC:{accuracy_score(yte.detach().numpy(),y_pred.detach().numpy()>0.
  ↪5)}') #classification
#y_pred, _, _=model_gd(Xte)
#performance metric for classification
```

```
#print(f'GD ACC:{accuracy_score(yte.detach().numpy(),y_pred.detach().numpy()>0.
↪5)}') #classification
y_pred, _, _=model_h(Xte)
#performance metric for classification
print(f'H  ACC:{accuracy_score(yte.detach().numpy(),y_pred.detach().numpy()>0.
↪5)}') #classification
#y_pred, _, _=model_ah(Xte)
#performance metric for classification
#print(f'AH ACC:{accuracy_score(yte.detach().numpy(),y_pred.detach().numpy()>0.
↪5)}') #classification
```

```
LS ACC:0.8
H  ACC:0.8206896551724138
```

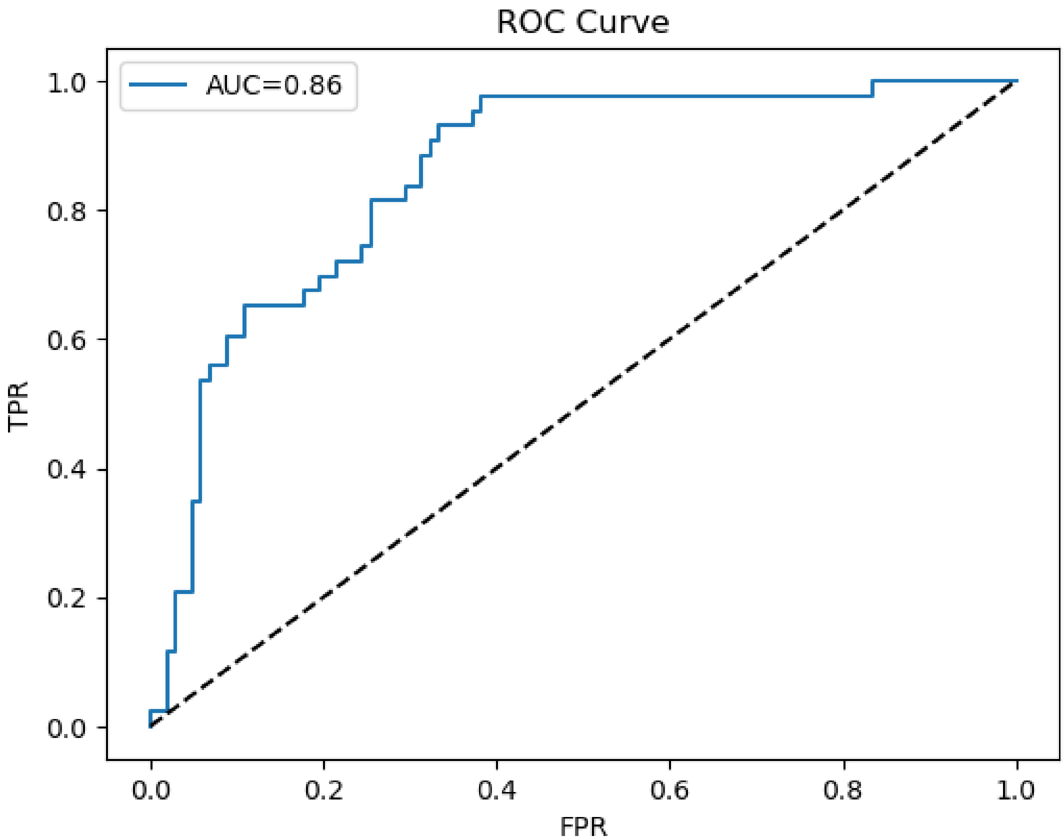
[22]:

```
# ---- forward pass on the test set ----
model_h.eval()
with torch.no_grad():
    Xte_t = Xte.float()
    logits, *_ = model_h(Xte_t)
    y_proba = torch.sigmoid(logits).cpu().numpy().reshape(-1)  # probabilities␣
↪in [0,1]

# ---- threshold at 0.5 to get class labels ----
y_pred = (y_proba > 0.5).astype(int)


# ---- confusion matrix ----
cm = confusion_matrix(yte, y_pred)
ConfusionMatrixDisplay(cm).plot(cmap="Blues")
plt.title("Confusion Matrix")
plt.show()
plt.savefig("../Plots/ConfusionMatrixANFIS.pdf", format="pdf",␣
↪bbox_inches="tight")
```



<Figure size 640x480 with 0 Axes>

[21]:
```
fpr, tpr, _ = roc_curve(yte, y_proba)
roc_auc = auc(fpr, tpr)
plt.plot(fpr, tpr, label=f"AUC={roc_auc:.2f}")
plt.plot([0,1],[0,1],'k--')
plt.xlabel("FPR"); plt.ylabel("TPR"); plt.title("ROC Curve"); plt.legend(); plt.
 ↪show()
plt.savefig("../Plots/RoCANFIS.pdf", format="pdf", bbox_inches="tight")
```




```
<Figure size 640x480 with 0 Axes>
```

[ ]: