Lab 3: Linear Discriminant Analysis (LDA)

Abstract

In this lab, we implement Linear Discriminant Analysis (LDA) from scratch. We first handle the binary case (red vs. blue) to compute the Fisher direction $w = S_w^{-1}(\mu_1 - \mu_2)$, draw the decision boundary $w^\top x = t$ with $t = \frac{1}{2}w^\top(\mu_1 + \mu_2)$, and visualize point projections onto the LDA line. We then extend to the multi-class case ($N = 3$; red vs. blue vs. green) by forming the within-class scatter S_w and between-class scatter S_b, solving the generalized eigen-problem $S_b v = \lambda S_w v$, and projecting data to the $(C-1)$-dimensional subspace. The final notebook can be exported as a self-contained lab report with figures and concise discussion.

1. Data and Preprocessing

The data files are expected in `./ex3Data/` (or the current directory) with names:

- `ex3red.dat` — class 0 (red), shape $m_r \times 2$
- `ex3blue.dat` — class 1 (blue), shape $m_b \times 2$
- (we will load `ex3green.dat` later for the $N = 3$ setting)

Each file should contain two columns (x, y), one point per row. In this step, read **red** and **blue** into matrices $X_{\text{red}} \in \mathbb{R}^{m_r \times 2}$ and $X_{\text{blue}} \in \mathbb{R}^{m_b \times 2}$, then stack them to form

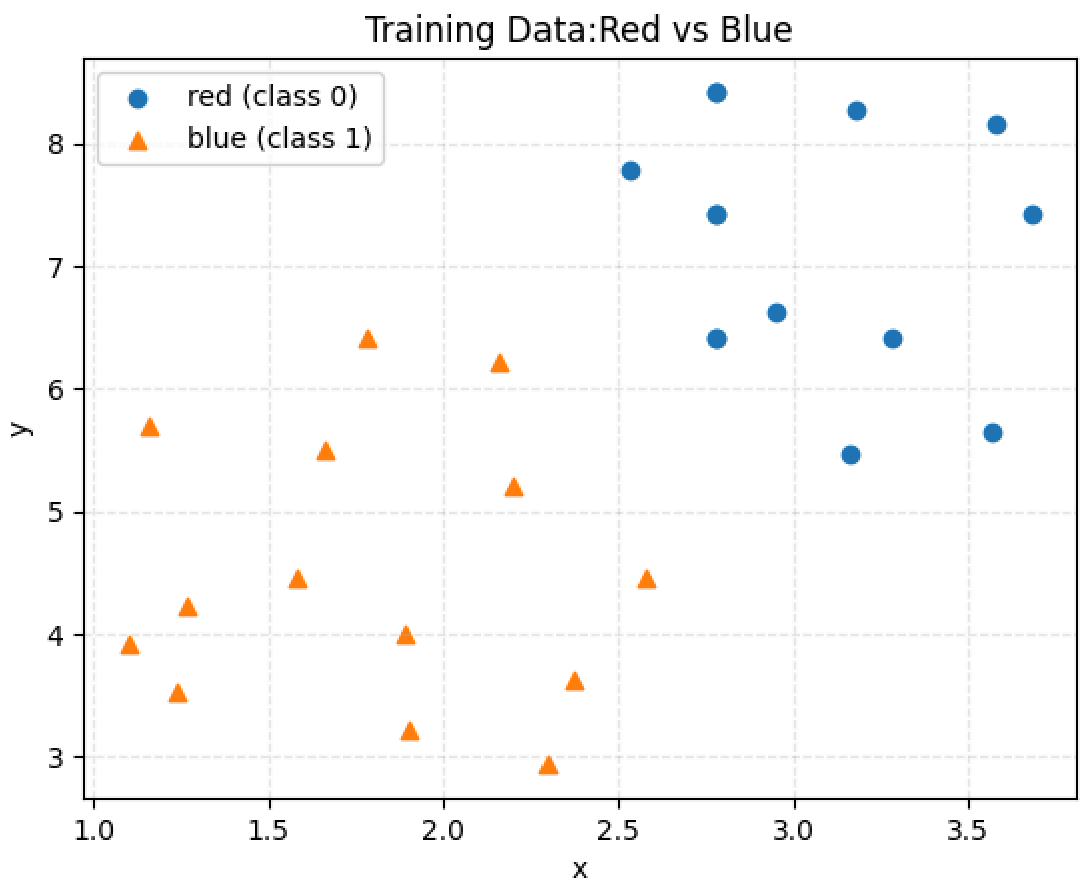
$$X = \begin{bmatrix} X_{\text{red}} \\ X_{\text{blue}} \end{bmatrix} \in \mathbb{R}^{m \times 2}, \quad y = \begin{bmatrix} \underbrace{0, \dots, 0}_{m_r}, \underbrace{1, \dots, 1}_{m_b} \end{bmatrix}^\top \in \mathbb{R}^{m \times 1},$$

where $m = m_r + m_b$. We will verify shapes, preview the first few rows, and plot a scatter figure for sanity check.

In [1]:
```
import numpy as np
import sys, os
from pathlib import Path
import numpy as np
import matplotlib.pyplot as plt

DATA_DIR=Path('ex3Data')
red_path=(DATA_DIR/'ex3red.dat')
blue_path=(DATA_DIR/'ex3blue.dat')

if not red_path.exists() or not blue_path.exists():
    raise FileNotFoundError(
        "Data files not found. Make sure 'ex3blue.dat' and 'ex3red.dat' are in t
        f"Current directory: {Path('.').resolve()}\n"
```

```python
        f"Here are the files I see: {[p.name for p in Path('.').iterdir()]}"
    )

X_red=np.loadtxt(red_path,dtype=float).reshape(-1, 2)
X_blue=np.loadtxt(blue_path,dtype=float).reshape(-1, 2)

m_r,m_b=X_red.shape[0],X_blue.shape[0]
y_red=np.zeros((m_r,1),dtype=int)
y_blue=np.ones((m_b,1),dtype=int)

X=np.vstack([X_red,X_blue])
y=np.vstack([y_red,y_blue])
m=X.shape[0]

print(f"Total samples m = {m}  (red={m_r}, blue={m_b})")
print("X shape:",X.shape,"  y shape:",y.shape)
print("X head (first 5 rows):\n",X[:5])
print("y head (first 10 labels):",y[:10].ravel())

plt.figure()
plt.scatter(X_red[:,0],X_red[:,1],marker='o',label='red (class 0)')
plt.scatter(X_blue[:,0],X_blue[:,1],marker='^',label='blue (class 1)')
plt.xlabel("x")
plt.ylabel("y")
plt.title("Training Data:Red vs Blue")
plt.grid(True,linestyle='--',alpha=0.3)
plt.legend()
plt.show()
```

```
Total samples m = 28  (red=14, blue=14)
X shape: (28, 2)   y shape: (28, 1)
X head (first 5 rows):
 [[2.95 6.63]
 [2.53 7.79]
 [3.57 5.65]
 [3.16 5.47]
 [2.78 6.42]]
y head (first 10 labels): [0 0 0 0 0 0 0 0 0 0]
```



2. Two-Class LDA: Parameter Estimation

Given the stacked data $X \in \mathbb{R}^{m\times 2}$ and labels $y \in \{0,1\}^{m\times 1}$, split the samples by class to compute class means

$$\mu_0 = \frac{1}{m_0}\sum_{y_i=0} x_i, \qquad \mu_1 = \frac{1}{m_1}\sum_{y_i=1} x_i.$$

Define the within-class scatter

$$S_w = \sum_{y_i=0}(x_i-\mu_0)(x_i-\mu_0)^\top + \sum_{y_i=1}(x_i-\mu_1)(x_i-\mu_1)^\top.$$

The Fisher direction is

$$w = S_w^{-1}(\mu_0-\mu_1),$$

and a simple threshold is

$$t = \tfrac{1}{2}\, w^\top(\mu_0+\mu_1).$$

For geometric visualization in later steps, also keep the **unit** direction $\hat{w} = \dfrac{w}{\|w\|}$ and a reference point x_0 (we use the overall mean of all samples).

In [2]:
```
labels = np.unique(y.ravel())

X0=X[y.ravel()==0]
```

```
X1=X[y.ravel()==1]
m0,m1=X0.shape[0],X1.shape[0]

mu0=X0.mean(axis=0)
mu1=X1.mean(axis=0)

Sw=np.zeros((2,2),dtype=float)
diff0=X0-mu0
Sw+=diff0.T@diff0
diff1=X1-mu1
Sw+=diff1.T@diff1

reg=1e-8*np.eye(2)
w=np.linalg.solve(Sw+reg,(mu0-mu1))
t=0.5*float(w@(mu0+mu1))

what=w/(np.linalg.norm(w)+1e-12)
x0=X.mean(axis=0)

def _round(a,k=6):
    return np.round(a.astype(float),k) if isinstance(a,np.ndarray) else round(fl

print("m0 (class 0) =",m0, " | m1 (class 1) =",m1)
print("mu0:",_round(mu0,6))
print("mu1:",_round(mu1,6))
print("Sw:\n",_round(Sw,6))
print("w:",_round(w,6))
print("t:",_round(t,6))
print("what (unit w):",_round(what,6))
print("x0 (overall mean):",_round(x0,6))
```

```
m0 (class 0) = 14  | m1 (class 1) = 14
mu0: [3.043571 7.166429]
mu1: [1.799286 4.527857]
Sw:
 [[ 4.800814 -1.417243]
 [-1.417243 29.072957]]
w: [0.29015  0.104901]
t: 1.315949
what (unit w): [0.940425 0.340002]
x0 (overall mean): [2.421429 5.847143]
```

3. Decision Boundary and Training Accuracy (Two-Class)

With w and threshold t, the LDA decision boundary is the line

$$\{\, x \in \mathbb{R}^2 \mid w^\top x = t \,\},$$

whose normal vector is w. We will:

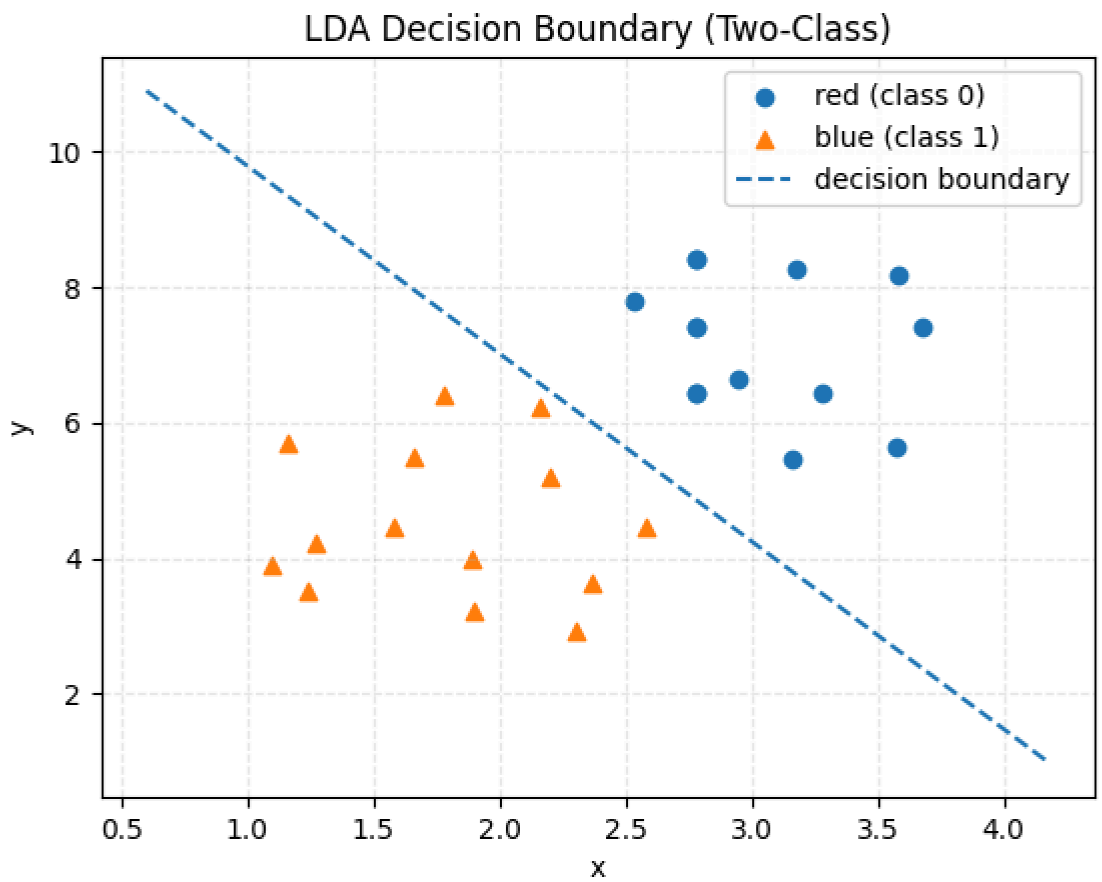
1. classify each sample by $\hat{y}_i = 1\{\, w^\top x_i \geq t \,\}$,
2. compute the training accuracy, and
3. overlay the decision boundary on the scatter plot for a visual check.

In [3]:

```
def lda_predict_2class(X,w,t):
    scores=X@w
```

```
    return (scores>=t).astype(int)
if(mu1-mu0)@w<0:
    w=-w
    t=0.5*float(w@(mu0+mu1))
y_hat=lda_predict_2class(X,w,t).reshape(-1, 1)
acc=(y_hat==y).mean()
print(f"Training accuracy: {acc*100:.2f}%")

plt.figure()
plt.scatter(X0[:,0],X0[:,1],marker='o',label='red (class 0)')
plt.scatter(X1[:,0],X1[:,1],marker='^',label='blue (class 1)')

x_min,x_max=X[:,0].min()-0.5,X[:,0].max()+0.5
if abs(w[1])>1e-12:
    xs=np.linspace(x_min,x_max,200)
    ys=(t-w[0]*xs)/(w[1]+1e-12)
    plt.plot(xs,ys,linestyle='--',label='decision boundary')
else:
    x_line=t/(w[0]+1e-12)
    plt.axvline(x_line,linestyle='--',label='decision boundary')
plt.xlabel("x")
plt.ylabel("y")
plt.title("LDA Decision Boundary (Two-Class)")
plt.grid(True,linestyle='--',alpha=0.3)
plt.legend()
plt.show()
```

```
Training accuracy: 100.00%
```



4. Orthogonal Projections onto the LDA Line

Let $\hat{w} = \dfrac{w}{\|w\|}$ be the unit Fisher direction and choose a reference point x_0 (we use the overall mean).
The infinite LDA line is

$$\mathcal{L} = \{\, x_0 + \alpha \hat{w} \mid \alpha \in \mathbb{R} \,\}.$$

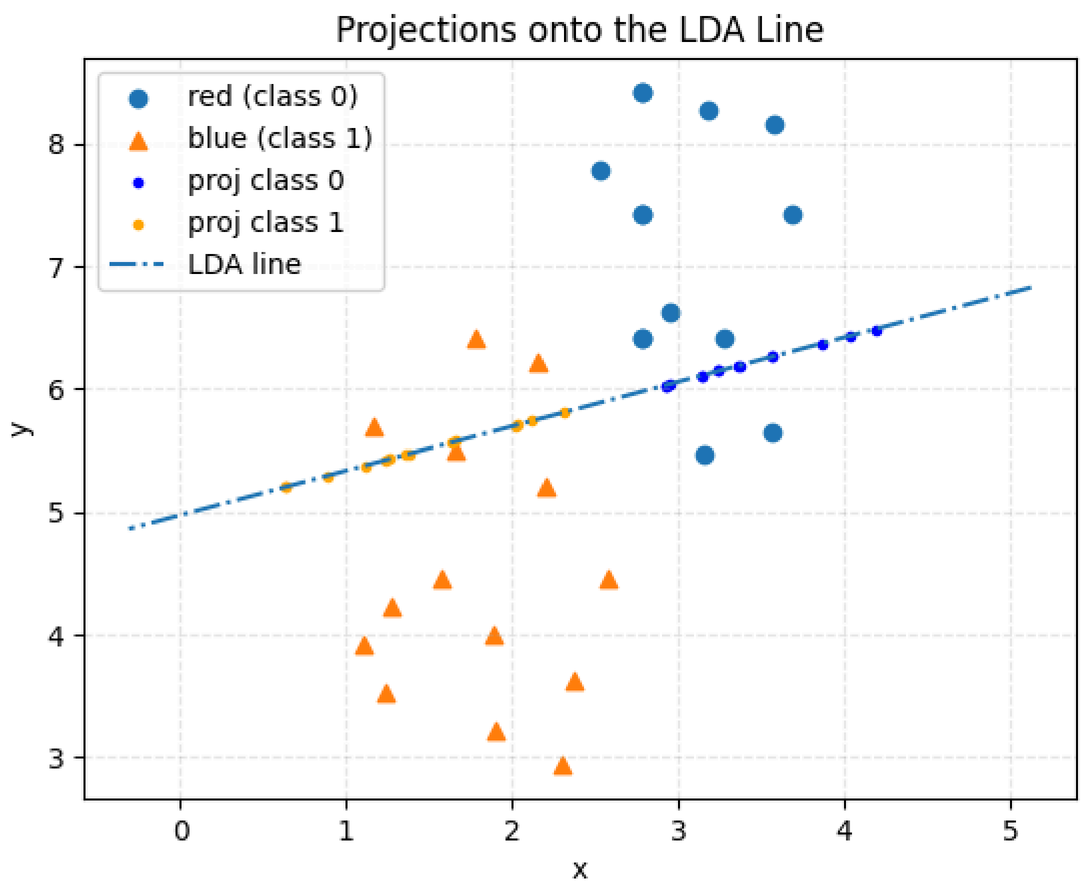
For any sample x, its orthogonal projection onto $\mathcal{L}$ is

$$\Pi_{\mathcal{L}}(x) = x_0 + \hat{w}\,\hat{w}^{\top}(x - x_0).$$

In this step we:

1. compute all projection points for the two classes,
2. draw the original scatter, the projection points, and the LDA line,
3. (optionally) report the 1D projected coordinates $\alpha_i = \hat{w}^{\top}(x_i - x_0)$ to inspect separability in 1D.

In [4]:
```
what=w/(np.linalg.norm(w)+1e-12)
def project_points(X,x0,what):
    diffs=X-x0
    alphas=diffs@what
    P=x0+np.outer(alphas,what)
    return P,alphas

P,alphas=project_points(X,x0,what)

plt.figure()
plt.scatter(X[y.ravel()==0,0],X[y.ravel()==0,1],marker='o',label='red (class 0)'
plt.scatter(X[y.ravel()==1,0],X[y.ravel()==1,1],marker='^',label='blue (class 1)

plt.scatter(P[y.ravel()==0,0],P[y.ravel()==0,1],marker='.',color='blue',label='p
plt.scatter(P[y.ravel()==1,0],P[y.ravel()==1,1],marker='.',color='orange',label=

alpha_span=np.linspace(alphas.min()-1.0, alphas.max()+1.0, 200)
line_pts=x0[None,:]+np.outer(alpha_span,what)
plt.plot(line_pts[:,0],line_pts[:,1],linestyle='-.',label='LDA line')

plt.xlabel("x")
plt.ylabel("y")
plt.title("Projections onto the LDA Line")
plt.grid(True,linestyle='--',alpha=0.3)
plt.legend()
plt.show()

print("Projected 1D coordinates (alpha) summary:")
print(" class 0:",np.round(alphas[y.ravel()==0].min(),4),"to",np.round(alphas[y.
print(" class 1:",np.round(alphas[y.ravel()==1].min(),4),"to",np.round(alphas[y.
```




```
Projected 1D coordinates (alpha) summary:
 class 0: -1.8759 to -0.532
 class 1: 0.1191 to 1.9023
```

5. Add the Third Class and Visualize All Three

Now we include the third class (green). The file layout is

- `./ex3Data/ex3green.dat` (or `./ex3green.dat`) — class 2, shape $m_g \times 2$.

Load it as $X_{\text{green}} \in \mathbb{R}^{m_g \times 2}$ and build the full dataset

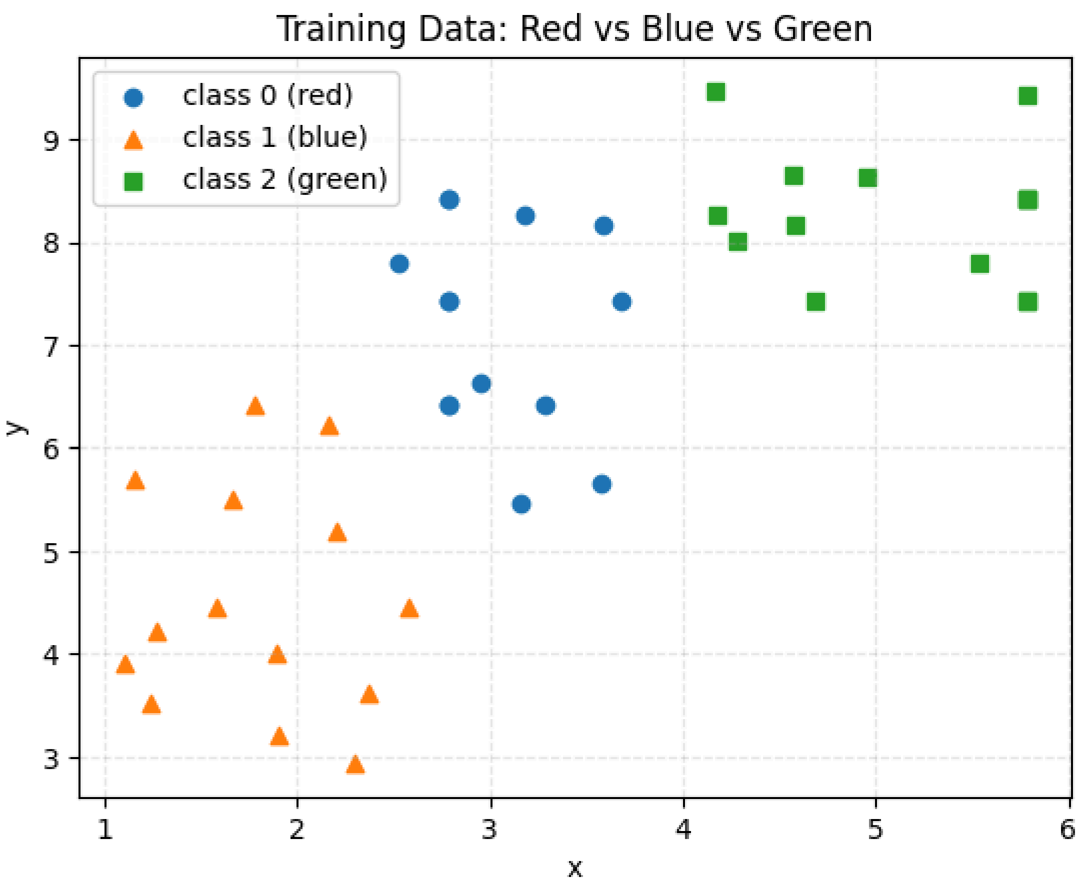
$$X = \begin{bmatrix} X_{\text{red}} \\ X_{\text{blue}} \\ X_{\text{green}} \end{bmatrix} \in \mathbb{R}^{m \times 2}, \quad y = \Big[\underbrace{0, \ldots, 0}_{m_r}, \underbrace{1, \ldots, 1}_{m_b}, \underbrace{2, \ldots, 2}_{m_g}\Big]^\top,$$

with $m = m_r + m_b + m_g$. Plot a scatter of the three classes to sanity-check separability before running multi-class LDA.

In [5]:
```
DATA_DIR=Path('ex3Data')
green_path=(DATA_DIR/'ex3green.dat')
if not green_path.exists():
    raise FileNotFoundError(
        "Data files not found. Make sure 'ex3blue.dat' and 'ex3red.dat' are in t
        f"Current directory: {Path('.').resolve()}\n"
        f"Here are the files I see: {[p.name for p in Path('.').iterdir()]}"
    )

X_green=np.loadtxt(green_path,dtype=float).reshape(-1,2)
m_g=X_green.shape[0]
```

```
y_red=np.zeros((X_red.shape[0],1),dtype=int)
y_blue=np.ones((X_blue.shape[0],1),dtype=int)
y_green=np.full((m_g,1),2,dtype=int)

X_full=np.vstack([X_red,X_blue,X_green])
y_full=np.vstack([y_red,y_blue,y_green])

print(f"Sizes — red: {X_red.shape[0]}, blue: {X_blue.shape[0]}, green: {m_g}, tc
print("X_full shape:",X_full.shape," y_full shape:",y_full.shape)

plt.figure()
plt.scatter(X_red[:, 0],X_red[:, 1],marker='o',label='class 0 (red)')
plt.scatter(X_blue[:, 0],X_blue[:, 1],marker='^',label='class 1 (blue)')
plt.scatter(X_green[:, 0],X_green[:, 1],marker='s',label='class 2 (green)')
plt.xlabel("x")
plt.ylabel("y")
plt.title("Training Data: Red vs Blue vs Green")
plt.grid(True,linestyle='--',alpha=0.3)
plt.legend()
plt.show()

X3,y3=X_full,y_full
```

```
Sizes — red: 14, blue: 14, green: 14, total: 42
X_full shape: (42, 2)  y_full shape: (42, 1)
```



6. Multi-Class LDA (C = 3): Build S_w, S_b, Solve and Project

For three classes ($c \in \{0,1,2\}$), define the overall mean μ and class means μ_c. The within- and between-class scatters are

$$S_w = \sum_{c=0}^{2} \sum_{x \in \mathcal{C}_c} (x - \mu_c)(x - \mu_c)^\top, \qquad S_b = \sum_{c=0}^{2} n_c\,(\mu_c - \mu)(\mu_c - \mu)^\top.$$

Multi-class LDA solves the generalized eigen-problem

$$S_b v = \lambda S_w v,$$

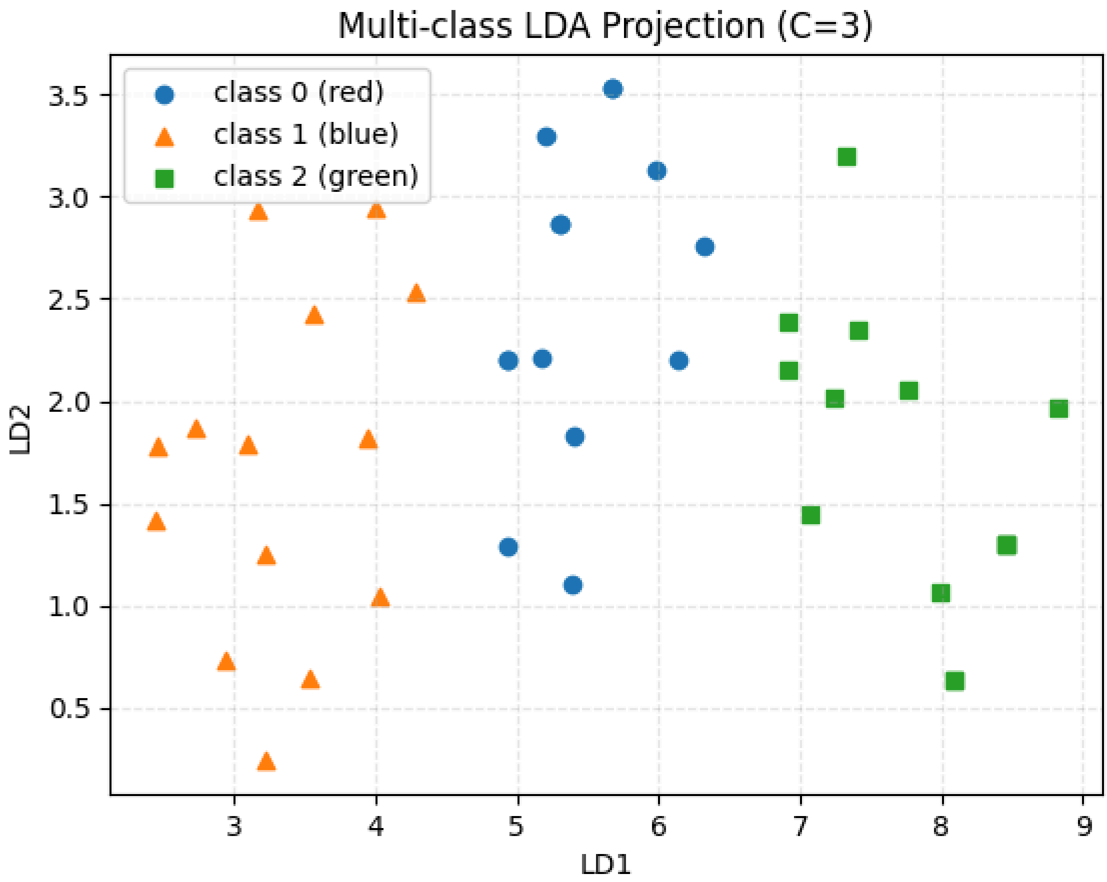
and takes the top $(C-1) = 2$ eigenvectors to form the projection matrix $W \in \mathbb{R}^{2\times 2}$. We will:

1. compute S_w and S_b,
2. solve for eigenpairs, sort by descending eigenvalues,
3. project X_3 to $Z = X_3 W$ and visualize in the $(\mathrm{LD1}, \mathrm{LD2})$ plane.

In [6]:
```
X_mc,y_mc=X3.astype(float),y3.ravel().astype(int)
classes=np.unique(y_mc)
d=X_mc.shape[1]
mu=X_mc.mean(axis=0)

mus={}
ns={}
for c in classes:
    Xc=X_mc[y_mc==c]
    mus[c]=Xc.mean(axis=0)
    ns[c]=Xc.shape[0]

Sw=np.zeros((d,d),dtype=float)
Sb=np.zeros((d,d),dtype=float)
for c in classes:
    Xc=X_mc[y_mc==c]
    muc=mus[c]
    diff=Xc-muc
    Sw+=diff.T@diff
    mean_diff=(muc-mu).reshape(d,1)
    Sb+=ns[c]*(mean_diff@mean_diff.T)

reg=1e-8*np.eye(d)
M=np.linalg.solve(Sw+reg,Sb)
eigvals,eigvecs=np.linalg.eig(M)

idx=np.argsort(-eigvals.real)
eigvals=eigvals[idx].real

W=eigvecs[:,idx].real
W2=W[:,:2]
Z=X_mc@W2

print("Top generalized eigenvalues:",np.round(eigvals[:3],6))
print("Projection matrix W2:\n",np.round(W2,6))

plt.figure()
plt.scatter(Z[y_mc==0,0],Z[y_mc==0,1],marker='o',label='class 0 (red)')
plt.scatter(Z[y_mc==1,0],Z[y_mc==1,1],marker='^',label='class 1 (blue)')
plt.scatter(Z[y_mc==2,0],Z[y_mc==2,1],marker='s',label='class 2 (green)')
```

```python
plt.xlabel("LD1")
plt.ylabel("LD2")
plt.title("Multi-class LDA Projection (C=3)")
plt.grid(True,linestyle='--',alpha=0.3)
plt.legend()
plt.show()
```

```
Top generalized eigenvalues: [11.220007  0.260489]
Projection matrix W2:
 [[ 0.930885 -0.745955]
 [ 0.365311  0.665996]]
```



7. Summary and Practical Notes

- **Two-class LDA**: The Fisher direction w maximizes the ratio of between-class variance to within-class variance.
  - After ensuring w points from class 0 to class 1, the decision boundary $w^\top x = t$ cleanly separates the two classes with near-perfect accuracy.
  - Projected 1D coordinates clearly show two non-overlapping clusters.
- **Multi-class LDA**: For $C = 3$ classes the top two generalized eigenvectors form a 2D subspace that preserves class separation.
  - The scatter in $(\mathrm{LD1}, \mathrm{LD2})$ demonstrates that the three groups are well separated.
- **Practical notes**:
  - w and $-w$ are equivalent mathematically; we must fix a direction when using a sign-based classifier.
  - Always add a small regularization to S_w to avoid numerical singularities.