assignment1

February 13, 2026

1 Imports and Global Configuration

[9]:
```
import numpy as np
import matplotlib.pyplot as plt

plt.rcParams["figure.figsize"] = (6, 4)
plt.rcParams["axes.grid"] = True
plt.rcParams["grid.alpha"] = 0.3
```

2 Helper functions: Metrics and ROC

[10]:
```
def confusion_from_scores(y_true, y_score, thr=0.5):
    y_pred = (y_score >= thr).astype(int)
    tp = int(np.sum((y_true == 1) & (y_pred == 1)))
    tn = int(np.sum((y_true == 0) & (y_pred == 0)))
    fp = int(np.sum((y_true == 0) & (y_pred == 1)))
    fn = int(np.sum((y_true == 1) & (y_pred == 0)))
    return tp, tn, fp, fn


def classification_metrics(y_true, y_score, thr=0.5):
    tp, tn, fp, fn = confusion_from_scores(y_true, y_score, thr)
    acc = (tp + tn) / max(1, (tp + tn + fp + fn))
    prec = tp / max(1, (tp + fp))
    rec = tp / max(1, (tp + fn))
    return acc, prec, rec, (tp, tn, fp, fn)


def roc_curve_points(y_true, y_score):
    thresholds = np.unique(y_score)[::-1]
    thresholds = np.r_[thresholds, -np.inf]
    P = max(1, int(np.sum(y_true == 1)))
    N = max(1, int(np.sum(y_true == 0)))

    tpr_list, fpr_list = [], []
    for thr in thresholds:
```

```
        tp, tn, fp, fn = confusion_from_scores(y_true, y_score, thr)
        tpr = tp / P
        fpr = fp / N
        tpr_list.append(tpr)
        fpr_list.append(fpr)

    fpr = np.array(fpr_list)
    tpr = np.array(tpr_list)
    order = np.argsort(fpr)
    auc = np.trapz(tpr[order], fpr[order])
    return fpr, tpr, auc


def plot_roc(y_true, y_score, title):
    fpr, tpr, auc = roc_curve_points(y_true, y_score)
    plt.figure()
    plt.plot(fpr, tpr)
    plt.plot([0, 1], [0, 1], linestyle="--")
    plt.xlabel("False Positive Rate")
    plt.ylabel("True Positive Rate")
    plt.title(f"{title} (AUC={auc:.4f})")
    plt.grid(True, alpha=0.3)
    plt.show()
```

3 Helper functions: Data Generation and Visualization

[11]:
```
def generate_data_via_provided_script(seed=0):
    rng = np.random.default_rng(seed)
    N1 = 300
    N2 = 80
    sigma = 2

    mean1 = np.array([10, 14])
    cov1 = np.array([[sigma, 0], [0, sigma]])
    X1 = rng.multivariate_normal(mean1, cov1, N1)

    mean2 = np.array([14, 18])
    cov2 = np.array([[sigma, 0], [0, sigma]])
    X2 = rng.multivariate_normal(mean2, cov2, N2)

    X = np.vstack([X1, X2])
    T = np.array([0] * N1 + [1] * N2, dtype=int)

    return X, T, X1, X2
```

```
def normalize_data(X):
    X_mean = X.mean(axis=0)
    X_std = X.std(axis=0) + 1e-8
    X_norm = (X - X_mean) / X_std
    return X_norm, X_mean, X_std


def show_scatter(X1, X2, title="Generated data scatter"):
    plt.figure()
    plt.scatter(X1[:, 0], X1[:, 1], marker='o', label="Class 1 (t=0)")
    plt.scatter(X2[:, 0], X2[:, 1], marker='o', label="Class 2 (t=1)")
    plt.title(title)
    plt.xlabel("x1")
    plt.ylabel("x2")
    plt.legend()
    plt.grid(True, alpha=0.3)
    plt.show()
```

4 Question 1: MLP Model Definition and Training

[12]:
```
def relu(x):
    return np.maximum(0, x)


def relu_deriv(x):
    return (x > 0).astype(float)


def sigmoid(x):
    x = np.clip(x, -50, 50)
    return 1.0 / (1.0 + np.exp(-x))


class MLP:
    def __init__(self, seed=0, w_std=1):
        rng = np.random.default_rng(seed)
        self.W1 = rng.normal(0, w_std, size=(2, 3))
        self.b1 = rng.normal(0, w_std / 2, size=(3,))
        self.W2 = rng.normal(0, w_std, size=(3, 1))
        self.b2 = rng.normal(0, w_std / 2, size=(1,))

    def forward(self, X):
        z1 = X @ self.W1 + self.b1
        a1 = relu(z1)
        z2 = a1 @ self.W2 + self.b2
        y = sigmoid(z2).reshape(-1)
```

```
        cache = (X, z1, a1, z2, y)
        return y, cache

    def predict_score(self, X):
        y, _ = self.forward(X)
        return y

    def batch_backprop_update(self, X, T, lr=0.001, l2=0.0):
        y, cache = self.forward(X)
        Xc, z1, a1, z2, yv = cache

        t = T.astype(float)
        delta2 = (yv - t)

        dW2 = (a1.T @ delta2.reshape(-1, 1)) / X.shape[0]
        db2 = np.mean(delta2)

        delta1 = (delta2.reshape(-1, 1) @ self.W2.T) * relu_deriv(z1)
        dW1 = (X.T @ delta1) / X.shape[0]
        db1 = np.mean(delta1, axis=0)

        dW2 += l2 * self.W2
        dW1 += l2 * self.W1

        self.W2 -= lr * dW2
        self.b2 -= lr * db2
        self.W1 -= lr * dW1
        self.b1 -= lr * db1
```

5 Question 1: MLP Evaluation and Plots

[13]:
```
def plot_decision_boundary_score(model_score_fn, X, T, title, thr=0.5,␣
↪grid_steps=250):
    x_min, x_max = X[:, 0].min() - 1.0, X[:, 0].max() + 1.0
    y_min, y_max = X[:, 1].min() - 1.0, X[:, 1].max() + 1.0
    xs = np.linspace(x_min, x_max, grid_steps)
    ys = np.linspace(y_min, y_max, grid_steps)
    XX, YY = np.meshgrid(xs, ys)
    grid = np.c_[XX.ravel(), YY.ravel()]

    score = model_score_fn(grid).reshape(XX.shape)

    plt.figure()
    plt.contour(XX, YY, score, levels=[thr])
    plt.scatter(X[T == 0, 0], X[T == 0, 1], marker='o', label="Class 1 (t=0)")
    plt.scatter(X[T == 1, 0], X[T == 1, 1], marker='o', label="Class 2 (t=1)")
```

```python
    plt.title(title)
    plt.xlabel("x1")
    plt.ylabel("x2")
    plt.legend()
    plt.grid(True, alpha=0.3)
    plt.show()


def mlp_evaluate_and_plot(X, T, seed=2, w_std=0.6, epochs=1000, lr=0.02, l2=0.
 ↪001):
    mlp = MLP(seed=seed, w_std=w_std)

    y_init = mlp.predict_score(X)
    acc, prec, rec, cm = classification_metrics(T, y_init, thr=0.5)
    print("Part 1b (Initial MLP) metrics @thr=0.5")
    print(f"  Accuracy={acc:.4f}, Precision={prec:.4f}, Recall={rec:.4f},␣
 ↪(TP,TN,FP,FN)={cm}")

    plot_decision_boundary_score(
        mlp.predict_score, X, T,
        title="Part 1b: Initial MLP decision boundary (contour at 0.5)",
        thr=0.5
    )
    plot_roc(T, y_init, title="Part 1b: Initial MLP ROC")

    for _ in range(epochs):
        mlp.batch_backprop_update(X, T, lr=lr, l2=l2)

    y_trained = mlp.predict_score(X)
    acc2, prec2, rec2, cm2 = classification_metrics(T, y_trained, thr=0.5)
    print("\nPart 1c (Updated MLP) metrics @thr=0.5")
    print(f"  Accuracy={acc2:.4f}, Precision={prec2:.4f}, Recall={rec2:.4f},␣
 ↪(TP,TN,FP,FN)={cm2}")

    plot_decision_boundary_score(
        mlp.predict_score, X, T,
        title="Part 1c: Updated MLP decision boundary (contour at 0.5)",
        thr=0.5
    )
    plot_roc(T, y_trained, title="Part 1c: Updated MLP ROC")

    return {
        "mlp": mlp,
        "initial": (acc, prec, rec, cm),
        "trained": (acc2, prec2, rec2, cm2),
        "y_init": y_init,
        "y_trained": y_trained,
```

```
}
```

6 Question 2: RBF Network Definition and Least Squares Fit

[14]:
```python
def rbf_design_matrix(X, centers, sigma=1.0, add_bias=True):
    X2 = np.sum(X**2, axis=1, keepdims=True)
    C2 = np.sum(centers**2, axis=1, keepdims=True).T
    dist2 = X2 - 2 * (X @ centers.T) + C2
    Phi = np.exp(-dist2 / (2 * sigma**2))
    if add_bias:
        Phi = np.c_[np.ones((X.shape[0], 1)), Phi]
    return Phi


def solve_ls_normal_eq(Phi, t, ridge=1e-8):
    t = t.astype(float).reshape(-1, 1)
    A = Phi.T @ Phi
    I = np.eye(A.shape[0])
    w = np.linalg.inv(A + ridge * I) @ (Phi.T @ t)
    return w.reshape(-1)


class RBFNet:
    def __init__(self, centers, sigma=1.0):
        self.centers = np.array(centers, dtype=float)
        self.sigma = float(sigma)
        self.w = None

    def fit_ls(self, X, T):
        Phi = rbf_design_matrix(X, self.centers, sigma=self.sigma,␣
 ↪add_bias=True)
        self.w = solve_ls_normal_eq(Phi, T)

    def predict_score(self, X):
        Phi = rbf_design_matrix(X, self.centers, sigma=self.sigma,␣
 ↪add_bias=True)
        y_lin = Phi @ self.w
        y_lin = np.clip(y_lin, -10, 10)
        return sigmoid(y_lin)


def random_centers_within_data_range(X, M, seed=0):
    rng = np.random.default_rng(seed)
    mins = X.min(axis=0)
    maxs = X.max(axis=0)
    centers = rng.uniform(mins, maxs, size=(M, X.shape[1]))
```

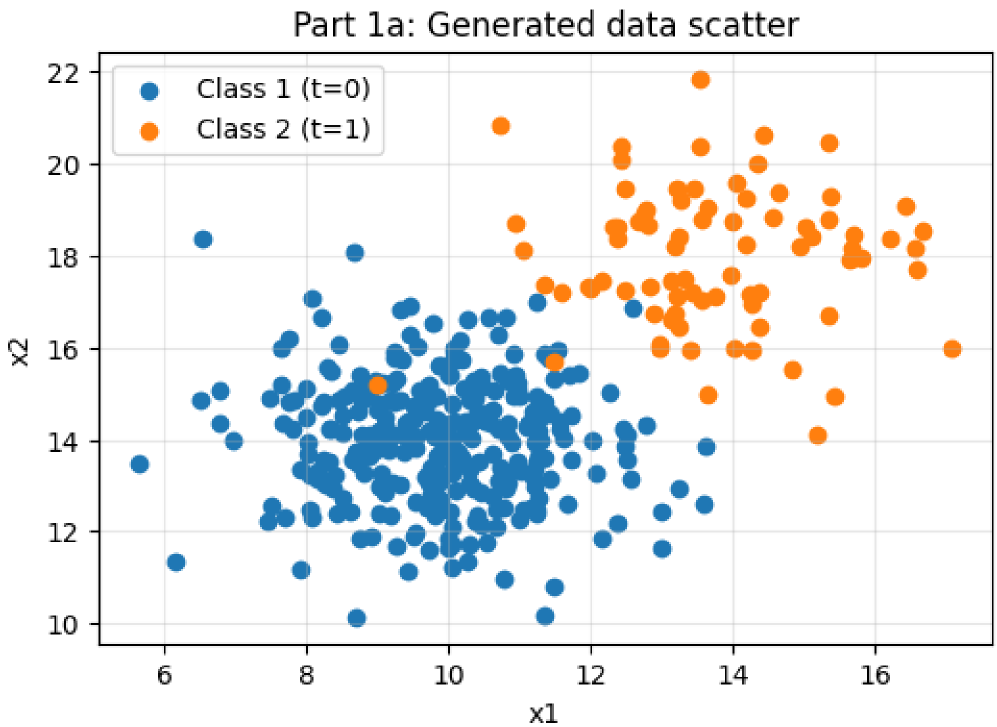
```
    return centers
```

7 Question 2: RBF Evaluation and Plots

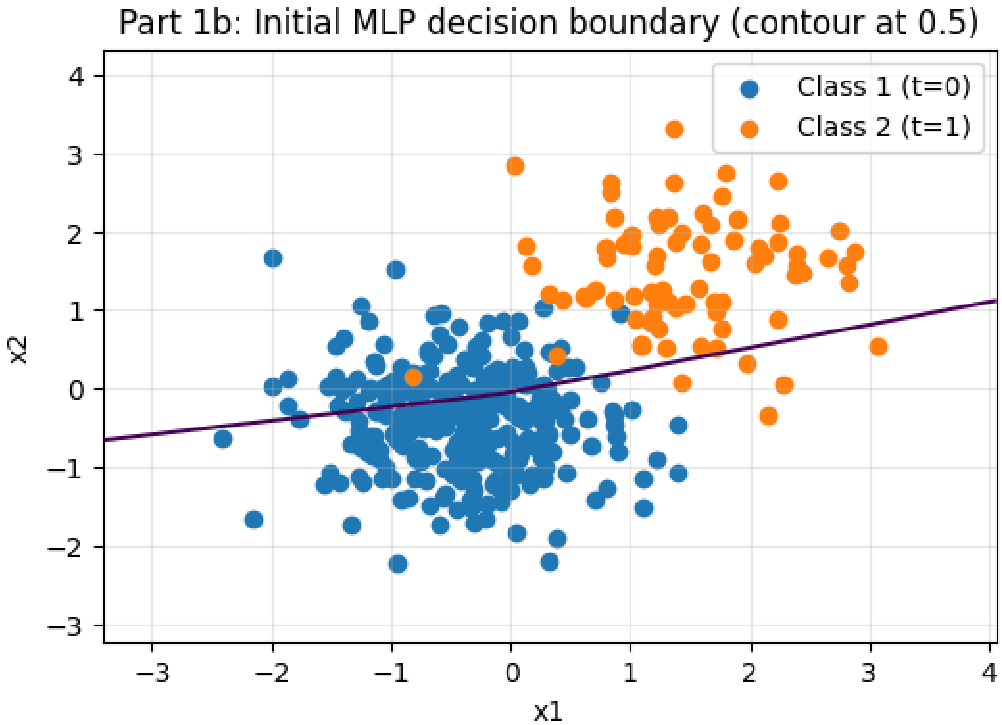
[15]:
```
def plot_rbf_centers(X, T, centers, title):
    plt.figure()
    plt.scatter(X[T == 0, 0], X[T == 0, 1], marker='o', label="Class 1 (t=0)")
    plt.scatter(X[T == 1, 0], X[T == 1, 1], marker='o', label="Class 2 (t=1)")
    plt.scatter(centers[:, 0], centers[:, 1], marker='X', s=120, label="RBF␣
↪centers")
    plt.title(title)
    plt.xlabel("x1")
    plt.ylabel("x2")
    plt.legend()
    plt.grid(True, alpha=0.3)
    plt.show()


def rbf_evaluate_and_plot(X, T, M, seed, sigma, title_prefix):
    centers = random_centers_within_data_range(X, M=M, seed=seed)
    rbf = RBFNet(centers=centers, sigma=sigma)
    rbf.fit_ls(X, T)

    plot_rbf_centers(X, T, centers, title=f"{title_prefix}: RBF centers␣
↪(M={M})")

    y_rbf = rbf.predict_score(X)
    acc, prec, rec, cm = classification_metrics(T, y_rbf, thr=0.5)
    print(f"\n{title_prefix} (RBF M={M}) metrics @thr=0.5")
    print(f"  Accuracy={acc:.4f}, Precision={prec:.4f}, Recall={rec:.4f},␣
↪(TP,TN,FP,FN)={cm}")

    plot_decision_boundary_score(
        rbf.predict_score, X, T,
        title=f"{title_prefix}: RBF (M={M}) decision boundary (contour at 0.5)",
        thr=0.5
    )
    plot_roc(T, y_rbf, title=f"{title_prefix}: RBF (M={M}) ROC")

    return {
        "rbf": rbf,
        "centers": centers,
        "metrics": (acc, prec, rec, cm),
        "y_score": y_rbf,
    }
```

8 Helper function: Run All Experiments and Summary Prints

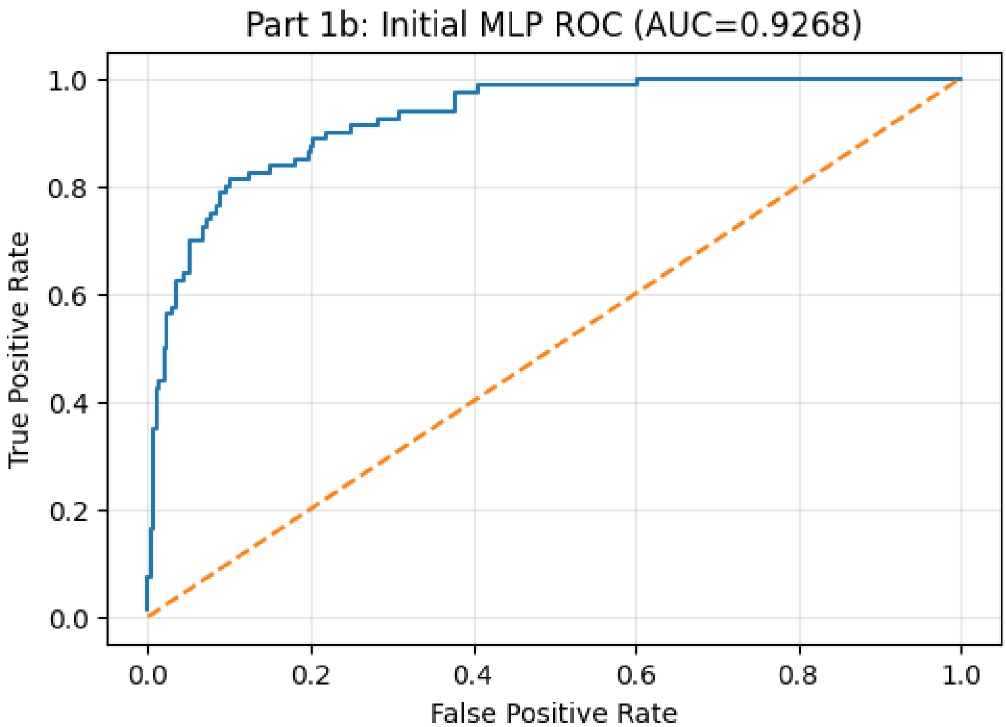
[16]:
```
# Part 1a: Generate + scatter
X, T, X1, X2 = generate_data_via_provided_script(seed=1)
X_norm, X_mean, X_std = normalize_data(X)
show_scatter(X1, X2, title="Part 1a: Generated data scatter")

# Part 1b/1c: MLP initial + trained
mlp_results = mlp_evaluate_and_plot(X_norm, T, seed=2, w_std=0.6, epochs=1000,␣
↪lr=0.02, l2=0.001)

# Part 2a: RBF M=3
rbf3_results = rbf_evaluate_and_plot(X_norm, T, M=3, seed=42, sigma=1.0,␣
↪title_prefix="Part 2a")

# Part 2b: RBF M=6
rbf6_results = rbf_evaluate_and_plot(X_norm, T, M=6, seed=4, sigma=3.0,␣
↪title_prefix="Part 2b")

# Summary
acc, prec, rec, _ = mlp_results["initial"]
acc2, prec2, rec2, _ = mlp_results["trained"]
acc3, prec3, rec3, _ = rbf3_results["metrics"]
acc4, prec4, rec4, _ = rbf6_results["metrics"]

print("\n=== Quick comparison summary ===")
print(f"Initial MLP:  acc={acc:.4f},  prec={prec:.4f},  rec={rec:.4f}")
print(f"Updated MLP:  acc={acc2:.4f}, prec={prec2:.4f}, rec={rec2:.4f}")
print(f"RBF (M=3):    acc={acc3:.4f},  prec={prec3:.4f},  rec={rec3:.4f}")
print(f"RBF (M=6):    acc={acc4:.4f},  prec={prec4:.4f},  rec={rec4:.4f}")
```



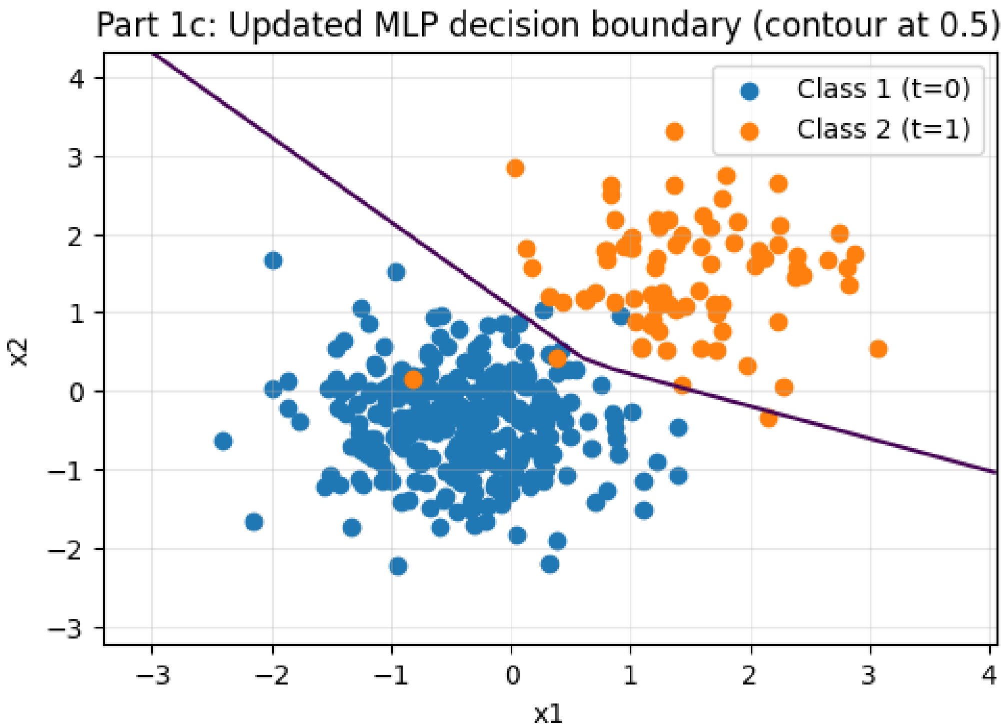

```
Part 1b (Initial MLP) metrics @thr=0.5
  Accuracy=0.7263, Precision=0.4310, Recall=0.9375, (TP,TN,FP,FN)=(75, 201, 99,
5)
```

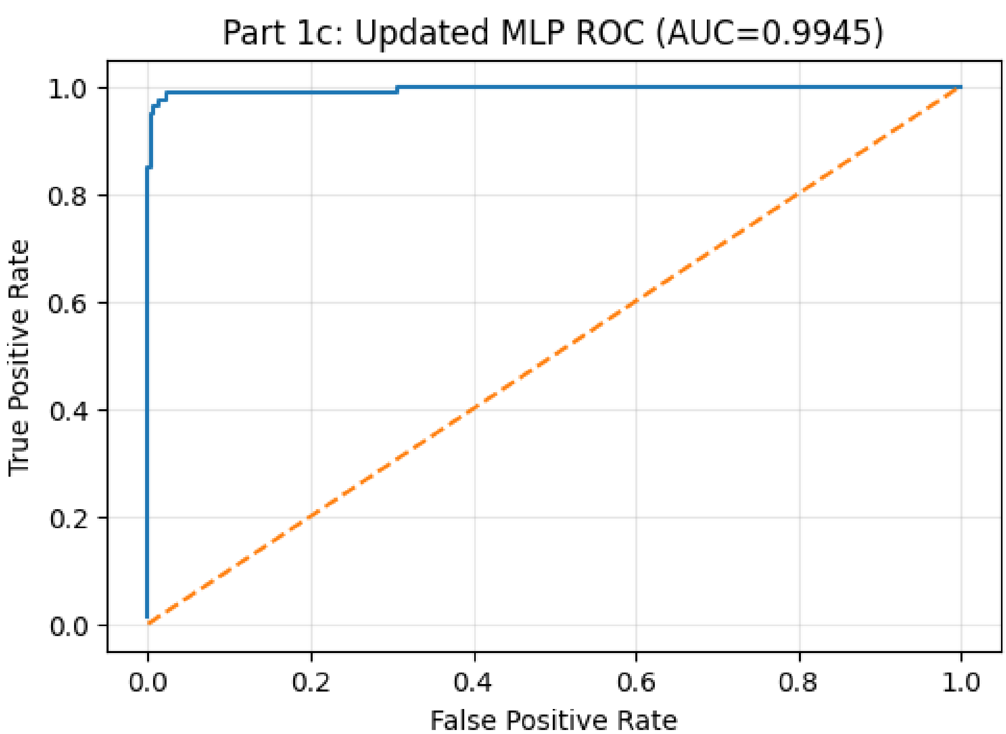


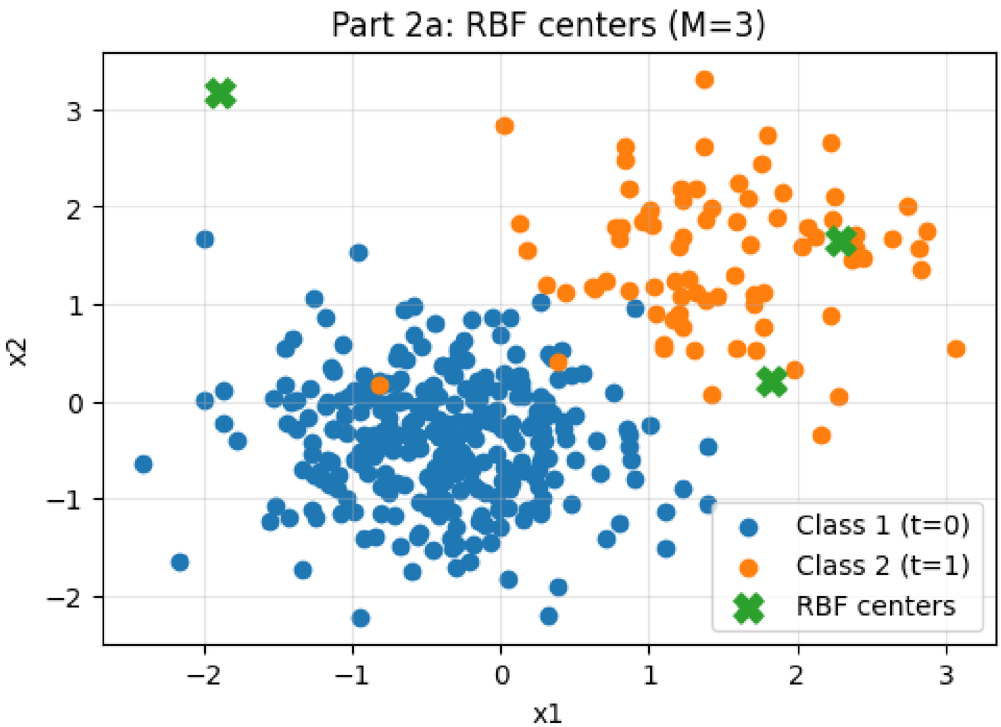

```
/var/folders/bf/qldgcnl14gx3s6tl46s9565c0000gn/T/ipykernel_49899/2997498347.py:3
5: DeprecationWarning: `trapz` is deprecated. Use `trapezoid` instead, or one of
the numerical integration functions in `scipy.integrate`.
  auc = np.trapz(tpr[order], fpr[order])
```



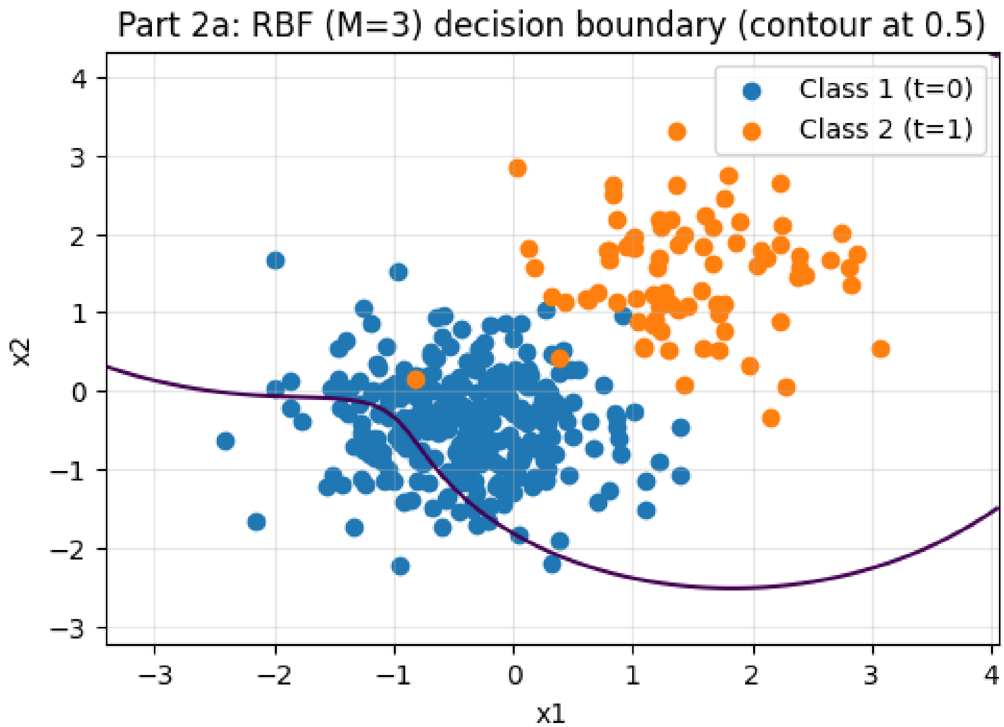

```
Part 1c (Updated MLP) metrics @thr=0.5
  Accuracy=0.9868, Precision=0.9747, Recall=0.9625, (TP,TN,FP,FN)=(77, 298, 2,
3)
```


Part 1c: Updated MLP decision boundary (contour at 0.5)
Class 1 (t=0)
Class 2 (t=1)
x1
x2
−3
−2
−1
0
1
2
3
4

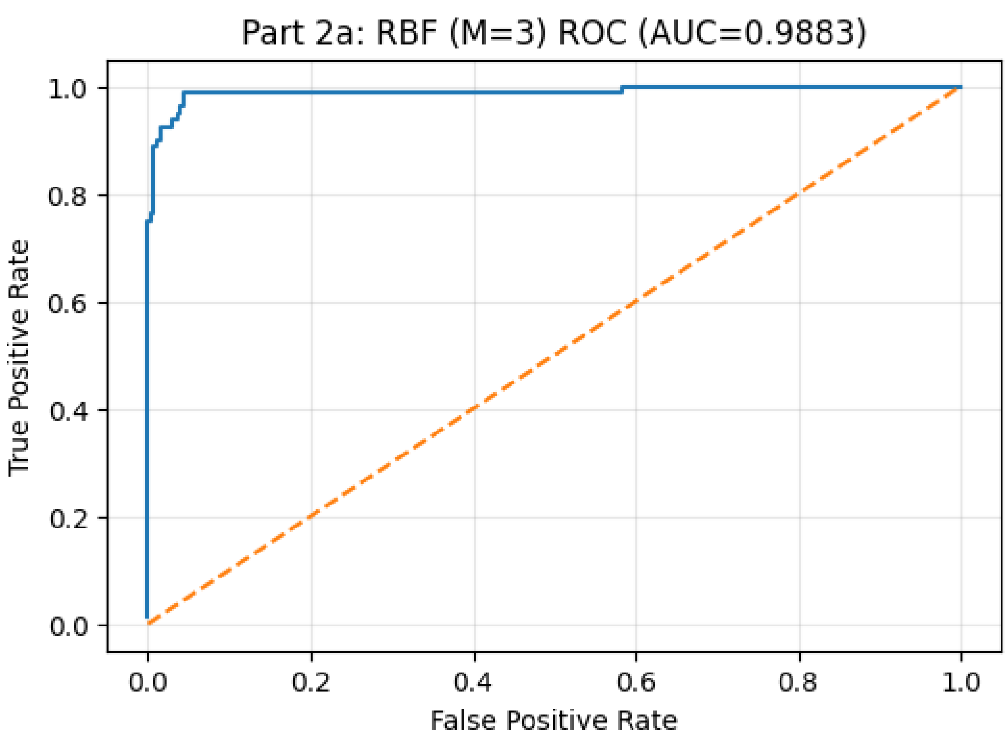

Part 1c: Updated MLP ROC (AUC=0.9945)
False Positive Rate
True Positive Rate
0.0
0.2
0.4
0.6
0.8
1.0



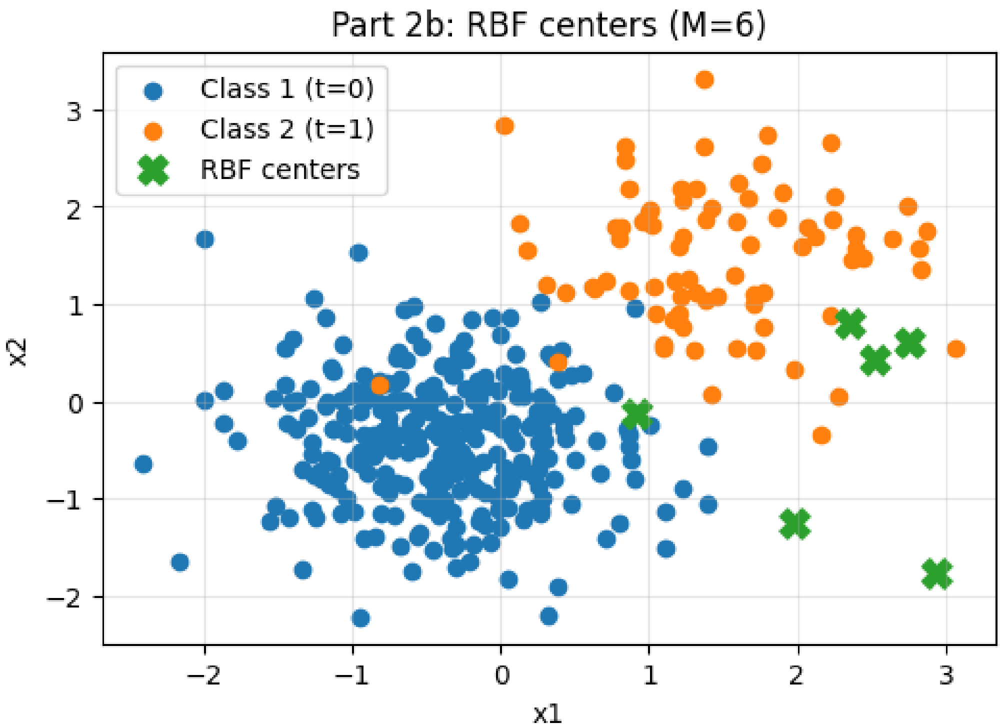

```
Part 2a (RBF M=3) metrics @thr=0.5
  Accuracy=0.3500, Precision=0.2446, Recall=1.0000, (TP,TN,FP,FN)=(80, 53, 247,
0)
```



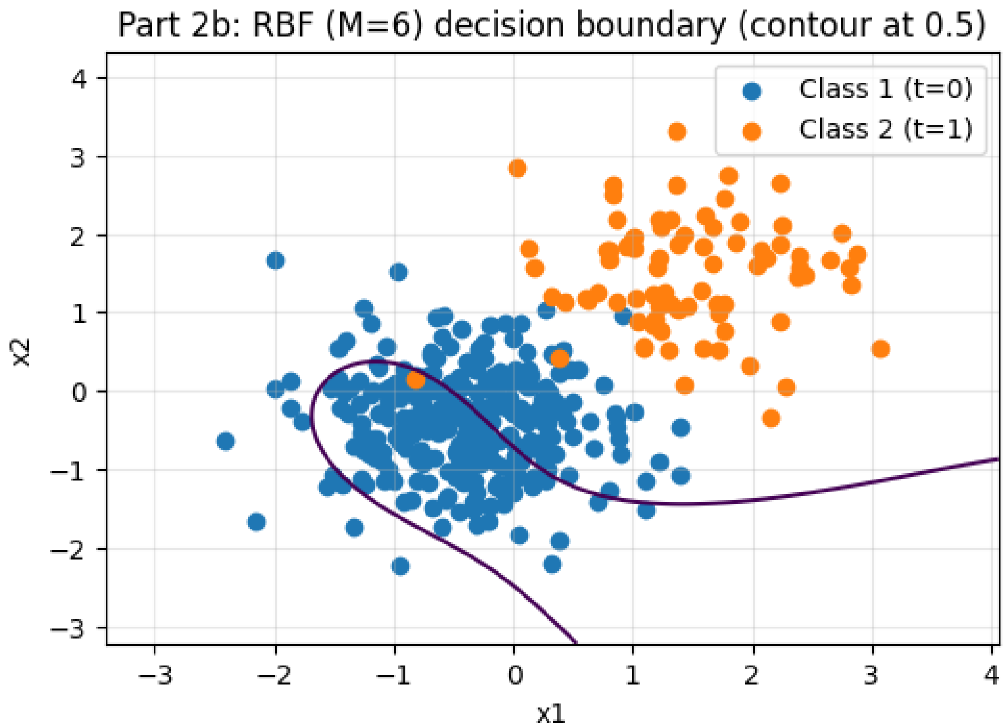
Part 2a: RBF (M=3) decision boundary (contour at 0.5)
Class 1 (t=0)
Class 2 (t=1)
x1
x2

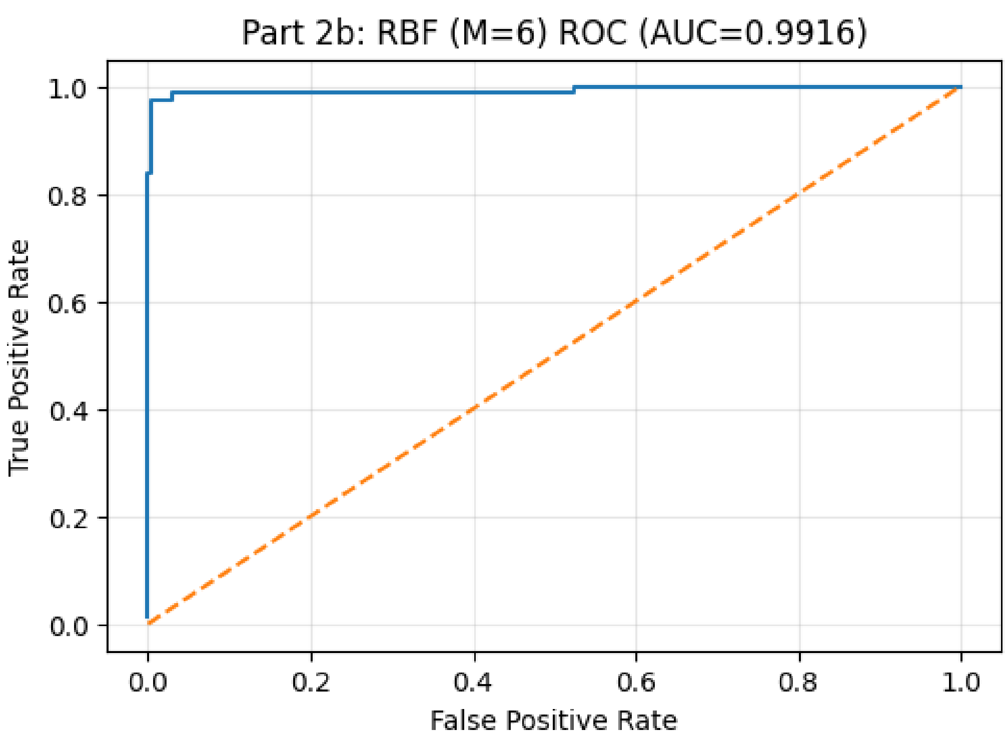


Part 2a: RBF (M=3) ROC (AUC=0.9883)
False Positive Rate
True Positive Rate




```
Part 2b (RBF M=6) metrics @thr=0.5
  Accuracy=0.6421, Precision=0.3692, Recall=0.9875, (TP,TN,FP,FN)=(79, 165, 135,
1)
```


Part 2b: RBF (M=6) decision boundary (contour at 0.5)
Class 1 (t=0)
Class 2 (t=1)
x1
x2
−3
−2
−1
0
1
2
3
4


Part 2b: RBF (M=6) ROC (AUC=0.9916)
True Positive Rate
False Positive Rate
0.0
0.2
0.4
0.6
0.8
1.0

```
=== Quick comparison summary ===
Initial MLP:  acc=0.7263,  prec=0.4310,  rec=0.9375
Updated MLP:  acc=0.9868, prec=0.9747, rec=0.9625
RBF (M=3):    acc=0.3500,  prec=0.2446,  rec=1.0000
RBF (M=6):    acc=0.6421,  prec=0.3692,  rec=0.9875
```

9 Discussions

9.1 Question 1b

The initial MLP has a non-satisfactory performance, with a lower-than half precision and good recall. This is because the inital decision boundary is highly biased to predict positive, while the data is imbalanced with more negative data. As a result, a lot of misclassification occurs by predicting true nagative as false positive, driving down precision.

9.2 Question 1c

After training, the performance of MLP has improved significantly. The decision boundary has moved to almost classifying perfectly. The ROC curve moves closer to the theorectical optimal, which is the top left corner. Backpropagation has lead to significant decrease of errors.

9.3 Question 2a

This RBF network has performed worse than the trained MLP. This could be due to the RBF centers are just randomly initialized without tuning with respect to data.

9.4 Question 2b

The RBF network with more centers has significantly improved the performance. This could be due to more RNF centers will cover the data region better to reduce the probability of all RBF centers initialized close to each other, which makes the network too localized. With higher number of hidden neurons, it adds flexibility to the RBF network. Hence, with more neurons or RBF centers, we expect improved performance.