Lecture 3: Linear Methods for Classification

Readings: ESL (Ch. 4, 12.1-12.2), ISL (Ch. 4); code

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September 2, 2025

Outline

The Classification Problem

Given a feature vector X, we want to predict a qualitative response G that takes values in a discrete set $\mathcal{G} = \{1, 2, \ldots, K\}$. We seek a classification rule (or classifier) $g(X)$ that assigns a class label to any input X.

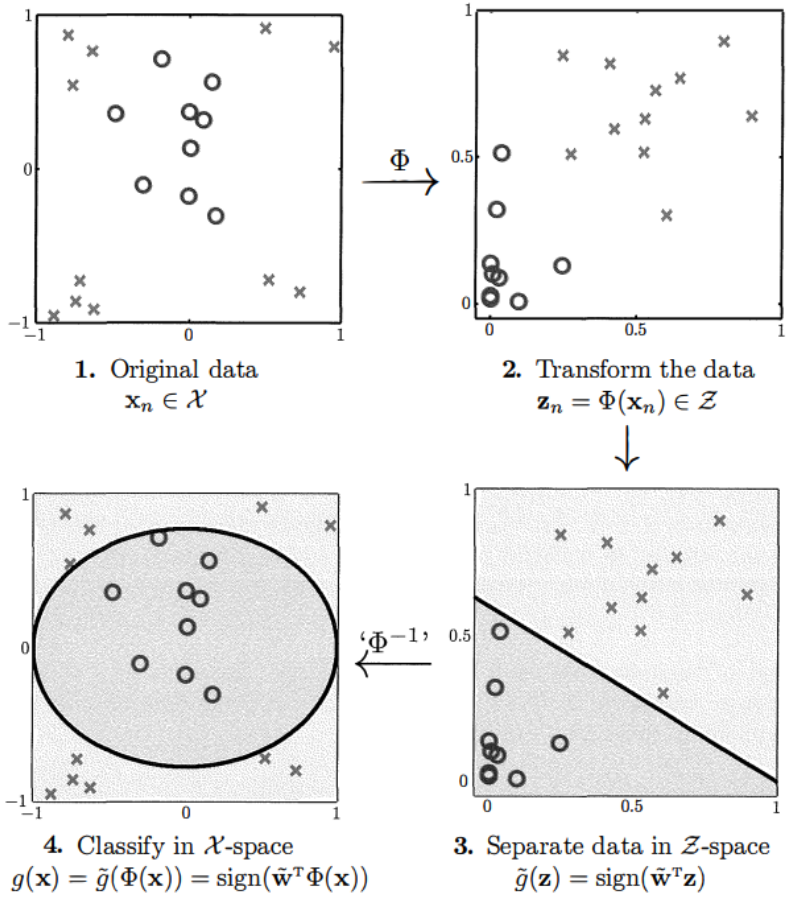
This lecture focuses on **linear methods for classification**, which produce **linear decision boundaries** in the input/feature space.

- A decision boundary is the surface in the input space that separates points assigned to different classes.
- For a linear classifier, these boundaries are affine sets/hyperplanes.
- Despite its simplicity, this is a powerful and widely used idea:

  
  Nonlinear boundaries can be achieved by augmenting the feature space with transformations (e.g., squares, cross-products) and then applying linear methods in the new enlarged space.

Example: Linearly Separable vs. Nonlinearly Separable

The data set is not linearly separable, but separable by a circle on the original input space. By mapping them to a suitable feature space, the transformed samples are linearly separable in the feature space.



Linear Classifiers

- For classification, the Bayes optimal classifier assigns an observation x to the class with the largest posterior probability $P(G = k|X = x)$.
- The decision boundary between two classes k and l is the set of points where the posterior probabilities are equal:

$$\{x \mid P(G = k|X = x) = P(G = l|X = x)\}.$$

⚠ Unlike LS regression, the ERM for classification rarely admits explicit solutions.

A Naive Method

Adapt linear regression for a classification problem.

Regression for Classification

1: If G has K classes, create an **indicator response matrix** $\mathbf{Y}$ of size $N \times K$, where $Y_{ik} = 1$ if observation i is in class k, and 0 otherwise.
2: Fit a multivariate linear regression model, regressing $\mathbf{Y}$ on $\mathbf{X}$. This gives the fit $\hat{\mathbf{Y}} = \mathbf{X}\hat{\mathbf{B}}$, where $\hat{\mathbf{B}} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{Y}$ is of size $(p+1) \times K$.
3: For a new input x, compute the vector of fitted values $\hat{f}(x)^T = (1, x^T)\hat{\mathbf{B}}$.
4: The classification rule is to choose the class with the largest fitted value:

$$\hat{G}(x) = \arg\max_{k \in \mathcal{G}} \hat{f}_k(x).$$

We can then view the regression as an estimate of conditional expectation: for the random variable Y_k, $\mathbb{E}[Y_k|X = x] = P(G = k|X = x)$.

Why This is (Usually) a Bad Idea

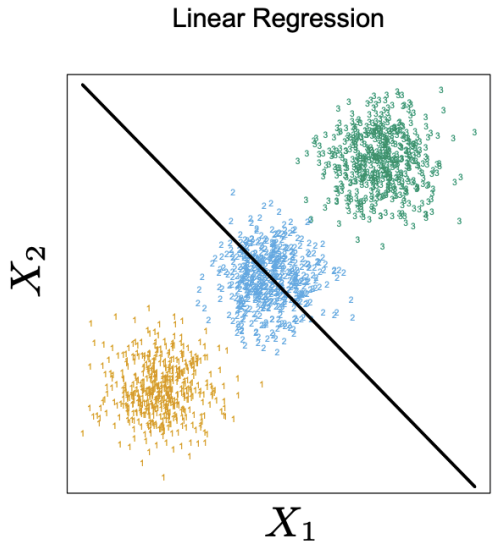
This approach seems simple, but it suffers from severe drawbacks.

1. Non-Probabilistic Predictions

- The fitted values $\hat{f}_k(x)$ are not probabilities.
- They are not constrained to be between 0 and 1.
- This makes interpretation difficult and can lead to unstable results.

2. The Masking Problem

- The rigid nature of the regression fit can lead to some classes being completely "masked" for $K \geq 3$ (natural for large K and small p).
- A decision region for a class might not exist, even if it is clearly present in the training data. This is a critical failure.



The Goal: The Bayes Optimal Classifier

The best possible classifier is the one that assigns an observation to the most probable class. This is the theoretical target we aim for.

Definition 1: The Bayes Optimal Classifier

Given the true class-conditional densities $f_k(x) = P(X = x|G = k)$ and priors $\pi_k = P(G = k)$, the class posterior probability is:

$$P(G = k|X = x) = \frac{\pi_k f_k(x)}{\sum_{l=1}^{K} \pi_l f_l(x)}.$$

The **Bayes classifier** classifies to the class with the highest posterior probability: $\hat{G}^*(x) = \arg\max_k P(G = k|X = x)$.

Since the true densities $f_k(x)$ and priors π_k are unknown, the Bayes optimal classifier cannot be implemented in practice. Instead, we use our training data to model or estimate them. **Different assumptions about the form of $f_k(x)$ lead to different classification methods.**

Three Approaches to Linear Classification

We will explore principled strategies for finding linear decision boundaries.

1. **Generative Approaches**
   - Model the class-conditional densities $P(X|G = k)$. Use Bayes' rule to compute the posteriors $P(G = k|X)$.
   - **Discriminant Analysis:** Assume each density is a multivariate Gaussian.
2. **Discriminative Approaches**
   - No assumption on $P(X|G)$, directly models the posterior probabilities $P(G = k|X)$.
   - **Logistic Regression:** Model the posterior probabilities directly as a logistic function.

3. **Direct Approaches** (don't model probabilities at all)
   - **Perceptron**: Rosenblatt's model and algorithm that finds a separating hyperplane in the data (if one exists).
   - **Support Vector Classifier (SVC):** Vapnik's method to find an optimal hyperplane that directly separates the data with a maximal margin.

Generative Approach: Linear Discriminant Analysis (LDA)

LDA is a generative approach that results from applying the Bayes' rule under specific assumptions about the form of the $f_k(x)$.

Definition 2: LDA Assumptions

1. The class-conditional probability density for each class, $f_k(x)$, is a **multivariate Gaussian**: $X|G = k \sim \mathcal{N}(\mu_k, \Sigma_k)$. The density is given by:

$$f_k(x) = \frac{1}{(2\pi)^{p/2}|\Sigma_k|^{1/2}} e^{-\frac{1}{2}(x-\mu_k)^T \Sigma_k^{-1}(x-\mu_k)}.$$

2. All classes share a **common covariance matrix**: $\Sigma_k = \Sigma \quad \forall k \in \mathcal{G}$.

Proposition 1: Decision Boundaries under LDA

Under the LDA assumptions, all the decision boundaries produced are linear.

Proof.

See blackboard. □

Deriving the LDA Decision Rule

We classify to the class that maximizes the log-posterior, $\log P(G = k|X = x)$. Since the denominator in Bayes' rule is the same for all classes, this is equivalent to maximizing:

$$\delta_k(x) = \log(\pi_k f_k(x)).$$

Substituting the Gaussian density with a common covariance matrix Σ:

$$\delta_k(x) = \log \pi_k - \frac{1}{2}\log((2\pi)^p|\Sigma|) - \frac{1}{2}(x-\mu_k)^T\Sigma^{-1}(x-\mu_k).$$

Expanding and dropping the terms that are constant across classes, we get the **linear discriminant function**:

$$\delta_k(x) = x^T\Sigma^{-1}\mu_k - \frac{1}{2}\mu_k^T\Sigma^{-1}\mu_k + \log \pi_k.$$

The classifier is given by $g(x) = \arg\max_k \delta_k(x)$ with $\delta_k(x)$ the above linear discriminant function.

Parameter Estimation for LDA

The parameters of the Gaussian model are estimated from the training data:

- **Priors:** $\hat{\pi}_k = N_k/N$, the proportion of training samples in class k.
- **Class Means:** $\hat{\mu}_k = \frac{1}{N_k} \sum_{g_i=k} x_i$, the average of the inputs for class k.
- **Common Covariance:** A pooled estimate of the covariance matrix:

$$\hat{\Sigma} = \frac{1}{N-K} \sum_{k=1}^{K} \sum_{g_i=k} (x_i - \hat{\mu}_k)(x_i - \hat{\mu}_k)^T.$$

These estimates are then plugged into the discriminant function to obtain $\hat{\delta}_k(x)$. The decision boundary between each pair of classes k and l is then described by $\{x : \hat{\delta}_k(x) = \hat{\delta}_l(x)\}$.

Connections to the Naive Approach

The Two-Class Case ($K = 2$)

For two classes, the least-squares regression approach is closely related to LDA:

- The direction of the decision boundary (orientation of the hyperplane) is identical to the LDA direction, up to a scaling factor (see Exercise 3.1).
- However, the intercept (the position of the boundary) is generally different. The two decision rules only coincide if the training classes have equal sizes.

The Multi-Class Case ($K \geq 3$)

- The methods are not equivalent. Linear regression on indicators can be severely compromised by "masking," where the model fails to separate certain classes.
- LDA finds the optimal subspace for discriminating between the class centroids, whereas the regression approach finds a suboptimal one.

Quadratic Discriminant Analysis (QDA)

QDA

- Like LDA, we assume $X|G = k \sim \mathcal{N}(\mu_k, \Sigma_k)$.
- Unlike LDA, we allow each class to have its own covariance matrix Σ_k.

When we derive the discriminant function, the quadratic term $x^T \Sigma_k^{-1} x$ **no longer cancels**:

$$\delta_k(x) = -\frac{1}{2} \log |\Sigma_k| - \frac{1}{2}(x - \mu_k)^T \Sigma_k^{-1}(x - \mu_k) + \log \pi_k.$$

The discriminant functions are now **quadratic** in x. This means the decision boundaries between classes are quadratic surfaces (conic sections like parabolas, hyperbolas, or ellipses).

QDA is more flexible than LDA but requires estimating many more parameters (esp. for large p), so it has higher variance.

LDA vs. QDA in Practice

- Both LDA and QDA have good track record, and perform well (likely due to the stability of the Gaussian model) on a large and diverse set of classification tasks.
- QDAs requires estimating $K \cdot p(p+1)/2$ covariance parameters, while LDA only requires $p(p+1)/2$.

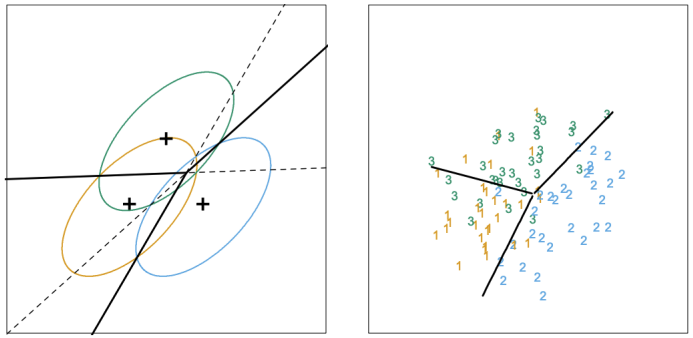


FIGURE 4.5. *The left panel shows three Gaussian distributions, with the same covariance and different means. Included are the contours of constant density enclosing 95% of the probability in each case. The Bayes decision boundaries between each pair of classes are shown (broken straight lines), and the Bayes decision boundaries separating all three classes are the thicker solid lines (a subset of the former). On the right we see a sample of 30 drawn from each Gaussian distribution, and the fitted LDA decision boundaries.*

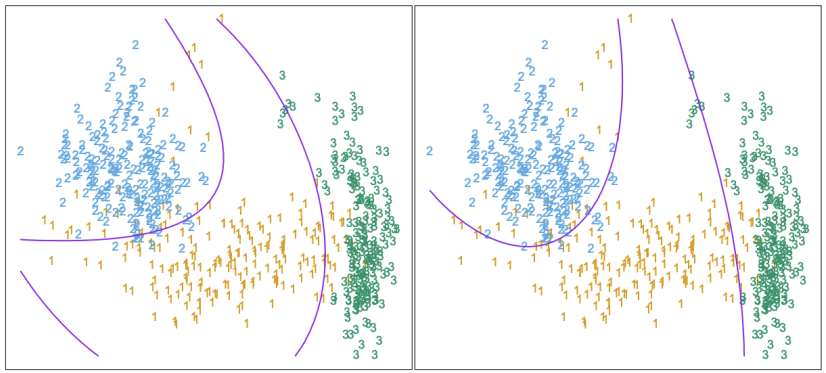


FIGURE 4.6. *Two methods for fitting quadratic boundaries. The left plot shows the quadratic decision boundaries for the data in Figure 4.1 (obtained using LDA in the five-dimensional space $X_1, X_2, X_1X_2, X_1^2, X_2^2$). The right plot shows the quadratic decision boundaries found by QDA. The differences are small, as is usually the case.*

Other Variants

Regularized Discriminant Analysis

A compromise between LDA and QDA that shrinks the separate covariances toward a common estimate, using the regularized covariance: $\hat{\Sigma}_k(\alpha) = \alpha\hat{\Sigma}_k + (1-\alpha)\hat{\Sigma}$.

- $\hat{\Sigma}_k$ is the covariance matrix of class k.
- $\hat{\Sigma}$ is the pooled covariance matrix (used in LDA).
- The tuning parameter $\alpha \in [0, 1]$ controls the amount of shrinkage.

Reduced-Rank Linear Discriminant Analysis

Performs dimension reduction by finding the linear combination $Z = a^T X$ that maximizes the ratio of between-class to within-class variance. This is achieved by solving Fisher's problem, maximizing the Rayleigh quotient $\max_a \frac{a^T \mathbf{B} a}{a^T \mathbf{W} a}$.

- $\mathbf{B}$ is the between-class covariance matrix of the class centroids.
- $\mathbf{W}$ is the pooled within-class covariance matrix.

The solutions v_ℓ are the eigenvectors from the generalized eigenvalue problem $\mathbf{B}v = \lambda \mathbf{W}v$. The resulting projections $Z_\ell = v_\ell^T X$ are the discriminant coordinates/canonical variates.

Discriminative Approach: Direct Probabilistic Models

- Instead of modeling $P(X|G)$ and using Bayes' rule (like LDA), directly models the posterior probabilities $P(G = k|X = x)$.
- This is a **discriminative** approach, as it focuses on the decision boundary without making assumptions about the distribution of the predictors.
- We focus on models that produce linear decision boundaries. If some monotone transformation ϕ of $P(G = k|X = x)$ is linear in x, then the decision boundaries produced are linear.
- A popular model is the **logistic regression model**, which uses the logit transformation.

The Logistic Model (Two Classes)

For two classes (labeled 0 and 1), let $p = P(G = 0|X = x)$ and take $\phi(p) = \log(p/(1-p))$ (the logit/log-odds). This gives the logistic regression model.

Definition 3: The Logit Model

$$\log \frac{P(G = 0|X = x)}{P(G = 1|X = x)} = \beta_0 + \beta^T x.$$

By inverting this transformation, we can express the probabilities directly. Since $P(G = 0|X) + P(G = 1|X) = 1$, we get:

$$P(G = 0|X = x) = \frac{e^{\beta_0+\beta^T x}}{1 + e^{\beta_0+\beta^T x}} = \frac{1}{1 + e^{-(\beta_0+\beta^T x)}},$$

$$P(G = 1|X = x) = \frac{1}{1 + e^{\beta_0+\beta^T x}}.$$

The decision boundary, where $P(G = 0|X) = P(G = 1|X) = 0.5$, occurs when $\beta_0 + \beta^T x = 0$, which is a hyperplane.

The Logistic Model (Multi-Class)

For $K > 2$ classes, the model is extended by picking one class as a baseline (e.g., class K) and modeling the log-odds of each other class relative to it.

Definition 4: The Multinomial Logit Model

For $k = 1, \ldots, K-1$:

$$\log \frac{P(G = k|X = x)}{P(G = K|X = x)} = \beta_{k0} + \beta_k^T x.$$

This gives the probabilities via the **softmax transformation**:

$$P(G = k|X = x) = \frac{e^{\beta_{k0} + \beta_k^T x}}{1 + \sum_{l=1}^{K-1} e^{\beta_{l0} + \beta_l^T x}} \quad \text{for } k = 1, \ldots, K-1.$$

And for the baseline class K:

$$P(G = K|X = x) = \frac{1}{1 + \sum_{l=1}^{K-1} e^{\beta_{l0} + \beta_l^T x}}.$$

The decision boundaries remain linear.

Fitting Logistic Regression via Maximum Likelihood

Fit the parameters by maximizing the conditional log-likelihood of G given X.

Definition 5: Log-Likelihood (Two-Class Case)

For N observations with a binary response $y_i \in \{0, 1\}$, the log-likelihood is:

$$\ell(\beta) = \sum_{i=1}^{N} \{y_i \log p(x_i; \beta) + (1 - y_i) \log(1 - p(x_i; \beta))\}$$

where $p(x_i; \beta) = P(G = 1 | X = x_i; \beta) = \frac{e^{\beta_{10} + \beta_1^T x_i}}{1 + e^{\beta_{10} + \beta_1^T x_i}}$ and $\beta = (\beta_{10}, \beta_1)$.
This is also known as the cross-entropy or binomial deviance.

- The log-likelihood is a **concave** function of β, which guarantees a unique maximum exists.
- No closed-form solution (why?) for the estimate $\hat{\beta}$: the solution must be found using an iterative algorithm like the **Newton-Raphson algorithm**.

The Newton-Raphson Algorithm (aka IRLS)

- Let $\mathbf{X}$ be the $N \times (p+1)$ design matrix, $\mathbf{y}$ be the vector of the y_i's, and $\mathbf{p}$ be the vector of fitted probabilities $p(x_i; \beta)$. The first and second derivatives are:

$$\frac{\partial \ell(\beta)}{\partial \beta} = \mathbf{X}^T(\mathbf{y} - \mathbf{p}) \quad \text{(Score vector)}$$

$$\frac{\partial^2 \ell(\beta)}{\partial \beta \partial \beta^T} = -\mathbf{X}^T\mathbf{W}\mathbf{X} \quad \text{(Hessian matrix)}$$

  where $\mathbf{W}$ is an $N \times N$ diagonal matrix with $W_{ii} = p(x_i; \beta)(1 - p(x_i; \beta))$.

- Starting with β^{old}, the updated estimate is:

$$\beta^{\text{new}} \leftarrow \beta^{\text{old}} - \left(\frac{\partial^2 \ell}{\partial \beta \partial \beta^T}\right)^{-1} \frac{\partial \ell}{\partial \beta}\bigg|_{\beta^{\text{old}}} = (\mathbf{X}^T\mathbf{W}\mathbf{X})^{-1}\mathbf{X}^T\mathbf{W}\mathbf{z},$$

  where $\mathbf{z} = \mathbf{X}\beta^{\text{old}} + \mathbf{W}^{-1}(\mathbf{y} - \mathbf{p})$ (adjusted response).

- This is a weighted least squares step for the $z_i = x_i^T \beta^{\text{old}} + \frac{y_i - p_i}{p_i(1-p_i)}$ (aka **Iteratively Reweighted Least Squares (IRLS)**).

Regularization for Logistic Regression

Regularization is crucial when p is large or when the data are separable, which can cause the MLE estimates to be undefined (why? see Exercise 3.2).

L2-Regularized (Ridge) Logistic Regression

Adds an L2 penalty to the log-likelihood:

$$\max_{\beta} \left\{ \ell(\beta) - \frac{\lambda}{2} \|\beta\|^2 \right\}.$$

Equivalent to placing a Gaussian prior on the coefficients in a Bayesian setting.

L1-Regularized (Lasso) Logistic Regression

Using an L1 penalty allows for feature selection:

$$\max_{\beta} \left\{ \ell(\beta) - \lambda \sum_{j=1}^{p} |\beta_j| \right\}.$$

This objective is still concave but the penalty is non-differentiable at zero.

The LDA and Logistic Regression Connection

There is a deep formal connection between LDA and logistic regression.

LDA's Posterior is a Logit Model

Under the LDA model's specific Gaussian assumptions, the log-odds between any two classes k and l is:

$$\log \frac{P(G=k|X=x)}{P(G=l|X=x)} = \log \frac{\pi_k}{\pi_l} - \frac{1}{2}(\mu_k + \mu_l)^T \Sigma^{-1}(\mu_k - \mu_l) + x^T \Sigma^{-1}(\mu_k - \mu_l).$$

This is a linear function of x, exactly like the logistic regression model:

$$\log \frac{P(G=k|X=x)}{P(G=l|X=x)} = \beta_{kl,0} + \beta_{kl}^T x.$$

Key Difference: LDA fits the parameters by maximizing the full log-likelihood based on the joint density $P(X, G)$, while logistic regression maximizes the conditional log-likelihood based on $P(G|X)$. The logistic model is more general as it doesn't assume Gaussian data.

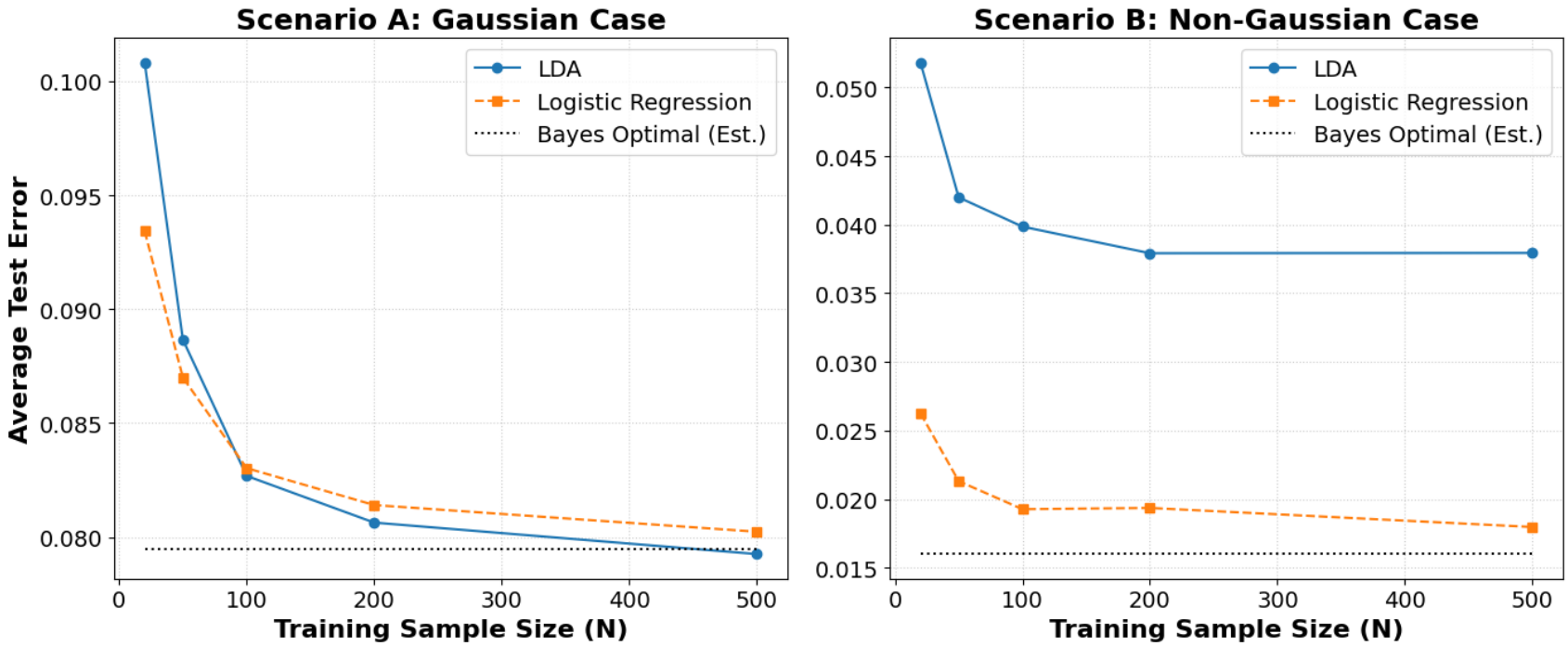
Summary: LDA vs. Logistic Regression

Both methods produce linear decision boundaries. How do they differ?

Linear Discriminant Analysis (LDA)	**Logistic Regression**
Generative model that models $P(X\|G)$ and $P(G)$.	Discriminative model that models $P(G\|X)$ directly.
Makes strong assumption that data is Gaussian with common covariance.	Makes minimal assumptions about the distribution of X.
More stable and efficient if the Gaussian assumption is met.	More robust and general. Often performs better if the LDA assumptions are not met but may need regularization.
Parameters found by maximizing the full log-likelihood (i.e., from moments).	Parameters found by maximizing the conditional log-likelihood.
Data points from all classes influence the boundary estimation.	Only the decision boundary matters; points far away from the boundary have little influence.

Example: LDA vs. Logistic Regression – Binary Case

- **Scenario A (Gaussian)**: Two Gaussian distributed classes with the same covariance matrix.
- **Scenario B (Non-Gaussian):** Class 0 is a mixture of two Gaussians, class 1 is a single Gaussian.



Direct Approaches: Construct Separating Hyperplanes

For a two-class problem with labels $y_i \in \{-1, 1\}$, consider linear classifiers of the form $\hat{g}(x) = \text{sign}(x^T\beta + \beta_0)$. The decision boundary is a hyperplane defined by $\{x : x^T\beta + \beta_0 = 0\}$.

Linearly Separable Data

If the training data is linearly separable, there exists at least one hyperplane that correctly classifies all training points, meaning $y_i(x_i^T\beta + \beta_0) > 0$ for all i.

❓ When the data are separable, there are infinitely many such hyperplanes. How do we find one? And which one should we choose?

- The **Perceptron Learning Algorithm** finds *a* separating hyperplane, if one exists.
- The **Optimal Separating Hyperplane** (Support Vector Classifier) finds the *best* one by maximizing the margin.

Rosenblatt's Perceptron Learning Algorithm

This algorithm attempts to find a separating hyperplane by minimizing the total distance of misclassified points to the decision boundary.

Definition 6: The Perceptron Criterion

The algorithm seeks to minimize:

$$D(\beta, \beta_0) = -\sum_{i \in \mathcal{M}} y_i (x_i^T \beta + \beta_0),$$

where $\mathcal{M}$ indexes the set of misclassfied points.
This criterion is non-negative and proportional to the sum of distances of the misclassified points to the boundary $x^T \beta + \beta_0 = 0$.

Note: the signed distance of a point x to the hyperplane $\{x : \beta^T x + \beta_0 = 0\}$ is given by $\frac{\beta^T x + \beta_0}{\|\beta\|}$ (check this). The sign indicates on which "side" of the hyperplane the point lies.

Perceptron Learning Algorithm

Perceptron Learning Algorithm

The algorithm uses stochastic gradient descent. For each misclassified point x_i in sequence, it updates the parameters:

$$\beta \leftarrow \beta + \rho \cdot y_i x_i$$
$$\beta_0 \leftarrow \beta_0 + \rho \cdot y_i$$

where ρ is the learning rate (typically set to 1).

- **Convergence:** For linearly separable data, it is guaranteed to converge to a separating hyperplane in a finite number of steps (Exercise 3.3).
- **Non-Uniqueness:** The solution found depends on the starting values. For separable data, there are many possible solutions.
- **Cycling:** If the data are *not* linearly separable, the algorithm will not converge and will cycle through different solutions.

Separating Hyperplanes and the Margin

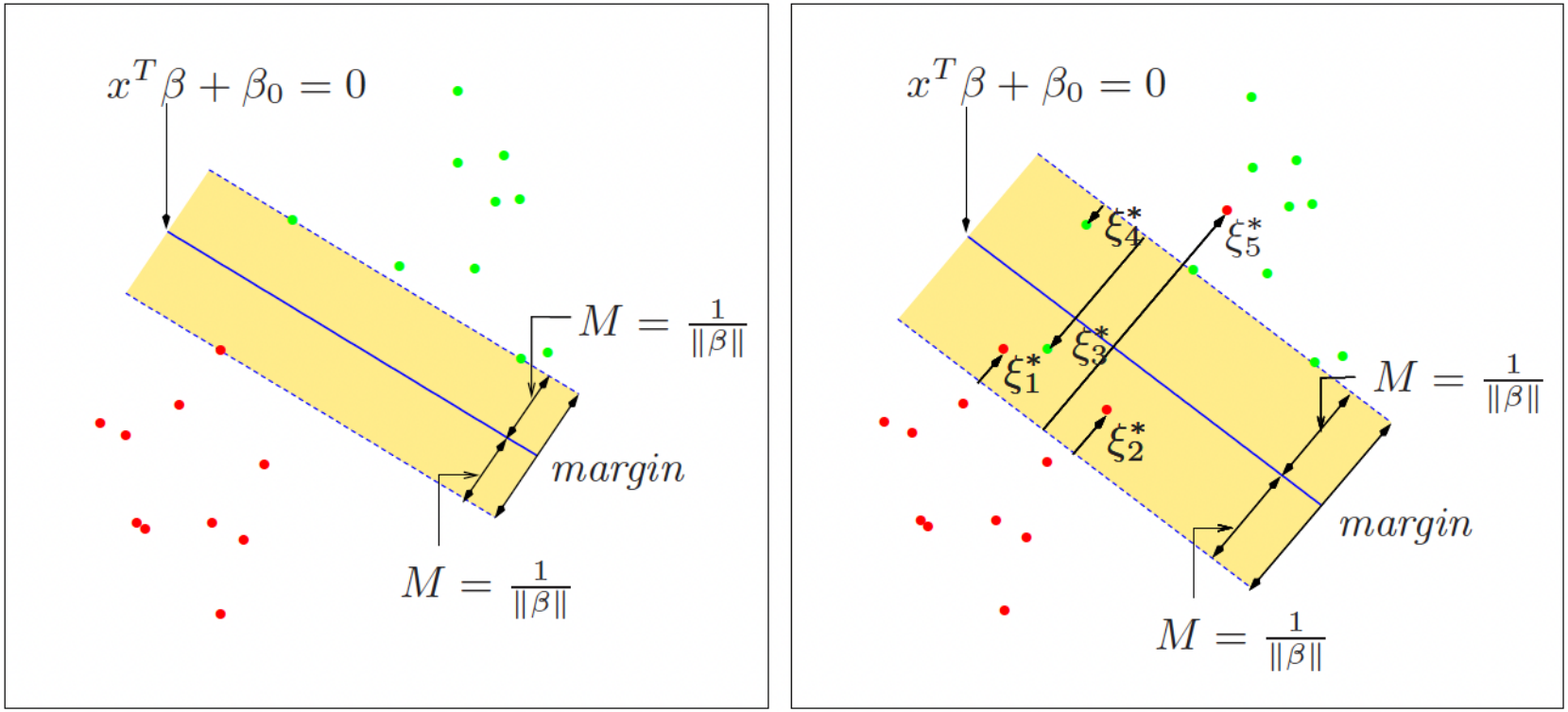


FIGURE 12.1. *Support vector classifiers. The left panel shows the separable case. The decision boundary is the solid line, while broken lines bound the shaded maximal margin of width* $2M = 2/\|\beta\|$. *The right panel shows the nonseparable (overlap) case. The points labeled* ξ_j^* *are on the wrong side of their margin by an amount* $\xi_j^* = M\xi_j$; *points on the correct side have* $\xi_j^* = 0$. *The margin is maximized subject to a total budget* $\sum \xi_i \leq$ *constant. Hence* $\sum \xi_j^*$ *is the total distance of points on the wrong side of their margin.*

Optimal Separating Hyperplanes: Maximizing the Margin

The optimal separating hyperplane uniquely solves the separability problem by maximizing the margin (the distance to the closest point from either class).

Definition 7: Maximizing the Margin (Separable Case)

We define the margin M and solve the optimization problem:

$$\max_{\beta,\beta_0,\|\beta\|=1} M \quad \text{subject to} \quad y_i(x_i^T\beta + \beta_0) \geq M, \ \forall i.$$

This is equivalent (why?) to minimizing $\|\beta\|^2$ subject to scaled constraints:

$$\min_{\beta,\beta_0} \frac{1}{2}\|\beta\|^2 \quad \text{subject to} \quad y_i(x_i^T\beta + \beta_0) \geq 1, \ \forall i.$$

The margin is then given by $M = 1/\|\beta\|$ (thickness). This is a convex optimization problem.

The Non-Separable Case: Introducing Slack Variables

To handle overlapping classes, we maximize M while allowing some points to be on the wrong side of the margin. Introduce the slack variables $\xi_i \geq 0$:

$$y_i(x_i^T \beta + \beta_0) \geq 1 - \xi_i, \quad \forall i,$$

and modify the optimization problem to be:

$$\min_{\beta, \beta_0, \xi} \frac{1}{2}\|\beta\|^2 + C\sum_{i=1}^{N} \xi_i \quad \text{s.t.} \quad \xi_i \geq 0, \; y_i(x_i^T \beta + \beta_0) \geq 1 - \xi_i \; \forall i. \tag{1}$$

- The parameter C is a cost parameter that controls the trade-off between maximizing the margin and the total error $\sum \xi_i$.
- Misclassifications occur when $\xi_i > 1$.
- See Exercise 3.4 for an equivalent problem as (1).

The Lagrange Dual Problem

The primal problem is a convex quadratic program with linear constraints.

The Wolfe Dual Problem. By maximizing the Lagrange dual function, we solve for the coefficients α_i. The dual problem is:

$$\max_{\alpha} \; L_D = \sum_{i=1}^{N} \alpha_i - \frac{1}{2} \sum_{i=1}^{N} \sum_{k=1}^{N} \alpha_i \alpha_k y_i y_k x_i^T x_k$$

subject to the constraints:

1. $0 \leq \alpha_i \leq C, \quad \forall i = 1, \ldots, N,$
2. $\sum_{i=1}^{N} \alpha_i y_i = 0.$

This is a simpler convex quadratic programming problem because the constraints are less complex than in the primal formulation. The solution for the weight vector β is recovered from the optimal $\hat{\alpha}_i$ values via $\hat{\beta} = \sum \hat{\alpha}_i y_i x_i$.

The Solution and Support Vectors

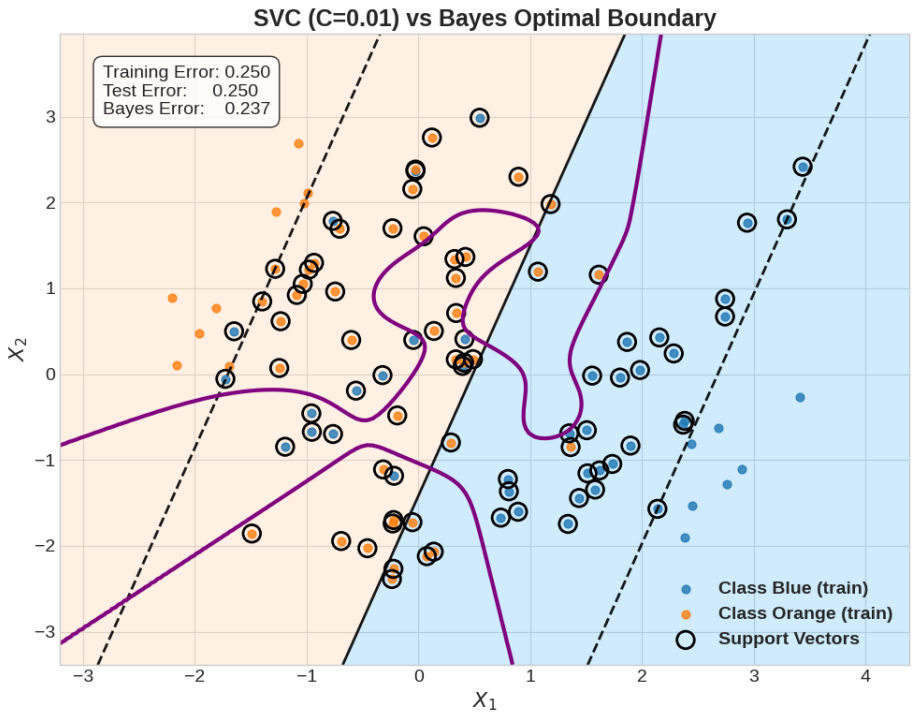
- The solution for the hyperplane vector β is a linear combination of the data points:

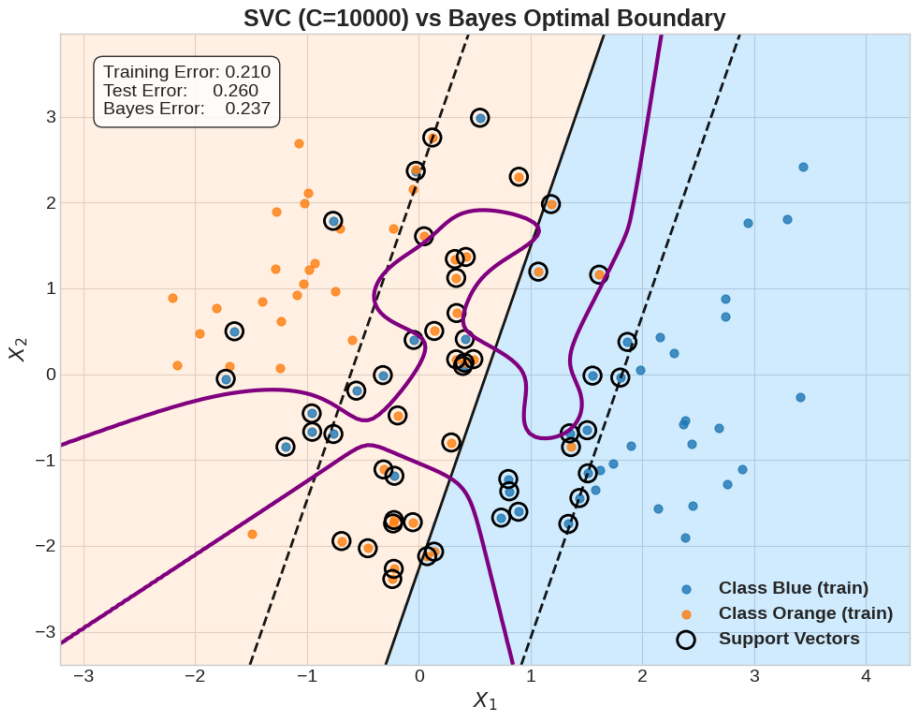
$$\hat{\beta} = \sum_{i=1}^{N} \hat{\alpha}_i y_i x_i.$$

- The Karush-Kuhn-Tucker (KKT) conditions imply that $\hat{\alpha}_i > 0$ only for observations x_i that lie on or inside the margin ($y_i(x_i^T \hat{\beta} + \hat{\beta}_0) \leq 1$). These points are called the **support vectors**.
- The final decision function is: $\hat{g}(x) = \text{sign}(x^T \hat{\beta} + \hat{\beta}_0)$. We call the model **support vector classifier (SVC)**.

None of the training data falls in the margin, but not necessarily for the test data. Key intuition is that a large margin on the training data will lead to good separation on the test data.

SVC: The Role of the Cost Parameter





- **Low C - High Regularization:**
  - Creates a **wide margin** by tolerating misclassifications.
  - Results in a simpler, high-bias boundary with fewer support vectors.
- **High C - Low Regularization:**
  - Creates a **narrow margin** to minimize training errors.
  - Give a more complex, high-variance boundary with many support vectors.

Optimal Separating Hyperplanes: Hard vs. Soft Margin

1. The Hard-Margin Classifier

- **Assumption:** The training data is perfectly, linearly separable.
- **Objective:** Find the hyperplane with the maximum possible margin.
- **Formulation:**

$$\min_{\beta,\beta_0} \frac{1}{2}\|\beta\|^2$$

subject to:

$$y_i(x_i^T\beta + \beta_0) \geq 1, \ \forall i.$$

- **Limitation:** Extremely sensitive to outliers and will fail if the data are not separable.

2. The Soft-Margin Classifier

- **Assumption:** The data may not be perfectly separable.
- **Objective:** Find a balance between a large margin and a low rate of margin violations.
- **Formulation:**

$$\min_{\beta,\beta_0,\xi} \frac{1}{2}\|\beta\|^2 + C\sum_{i=1}^{N}\xi_i$$

subject to:

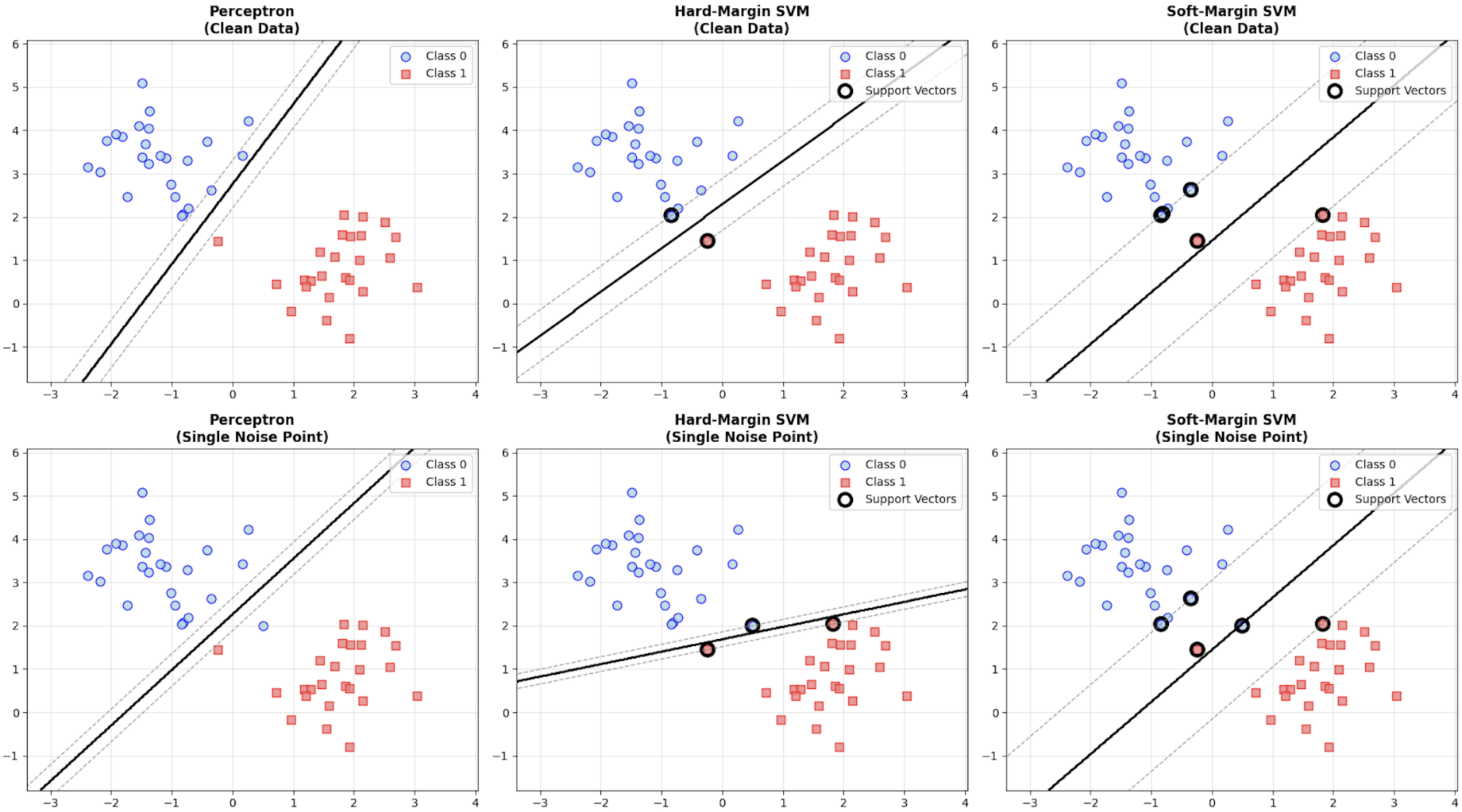
$$y_i(x_i^T\beta + \beta_0) \geq 1 - \xi_i, \ \xi_i \geq 0.$$

- **Robustness:** The cost parameter C controls the trade-off, making the classifier robust to outliers.

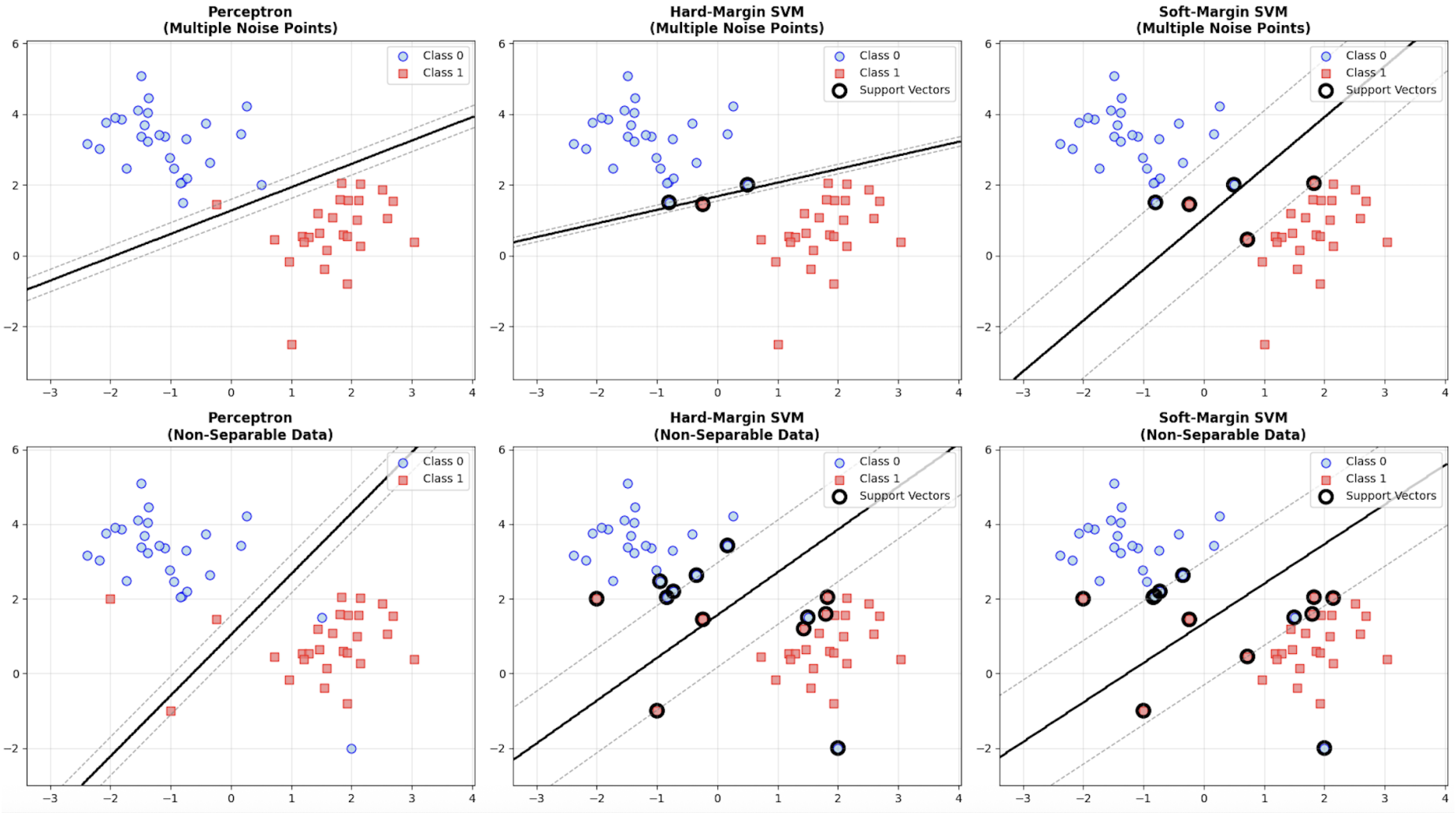
Perceptron vs. SVCs: Robustness to Noise

- **Data:** Generate a small, linearly separable two-class dataset.
- **Step 1:** Fit three models on clean data:
  (1) Perceptron (finds any separating hyperplane),
  (2) Hard-Margin SVC ($C = 10^6$, maximizes margin),
  (3) Soft-Margin SVC ($C = 1.0$, allows some misclassifications).
- **Step 2:** Test robustness under three noise scenarios:
  - Add a single noisy data point near the decision boundary
  - Add multiple noisy outlier points in different regions
  - Create non-separable data by adding points with conflicting class labels
- **Step 3:** Re-fit all models on each noisy dataset and compare:
  - Decision boundary stability and changes
  - Support vector identification (for SVCs)
  - Margin visualization and robustness
  - Classification accuracy on each scenario

Empirical Results



Empirical Results



A Unifying View: Loss + Penalty

The classification and regression models we have seen so far can be understood through a single, powerful framework.

Definition 8: The "Loss + Penalty" Framework

The goal is to find the function f that minimizes:

$$\sum_{i=1}^{N} \underbrace{L(y_i, f(x_i))}_{\text{Loss Function}} + \lambda \underbrace{J(f)}_{\text{Penalty Term}} .$$

Model	**Loss Function** $L(y, f(x))$	**Penalty** $J(f)$
Ridge Regression	$(y - f(x))^2$	$\|\beta\|_2^2$
Lasso Regression	$(y - f(x))^2$	$\|\beta\|_1$
Logistic Regression	$\log(1 + e^{-yf(x)})$	$\|\beta\|_2^2$ (Ridge) or $\|\beta\|_1$ (Lasso)
SVC	$[1 - yf(x)]_+$ (Hinge Loss)	$\|\beta\|_2^2$

Exercises

Exercise 3

1. Solve Exercise 4.2 in ESL.
2. Solve Exercise 4.5 in ESL.
3. Solve Exercise 4.6 in ESL.
4. For $f(x) = x^T\beta + \beta_0$, consider the optimization problem:

$$\min_{\beta_0,\beta} \sum_{i=1}^{N} [1 - y_i f(x_i)]_+ + \frac{\lambda}{2}\|\beta\|^2, \tag{2}$$

where "+" indicates positive part. Show that the solution to the above problem (with $\lambda = 1/C$), is the same as that for (1).

Exercises

Exercise 3 (experimental)

Generate a 2D synthetic dataset with two classes ($Y = 0$ and $Y = 1$), each following a multivariate Gaussian distribution: $X|Y = 0 \sim \mathcal{N}(\mu_0, \Sigma_0)$, $X|Y = 1 \sim \mathcal{N}(\mu_1, \Sigma_1)$, where $\mu_0 = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$, $\Sigma_0 = \begin{bmatrix} 1 & 0.5 \\ 0.5 & 1 \end{bmatrix}$, $\mu_1 = \begin{bmatrix} 2 \\ 2 \end{bmatrix}$, $\Sigma_1 = \begin{bmatrix} 1 & -0.3 \\ -0.3 & 1 \end{bmatrix}$. Generate 200 samples per class and then split the data into training (70%) and test sets (30%).

1. Implement a classification model using: LDA, QDA, logistic regression, perceptron and SVC. Fit each model on the training data and compute the misclassification error on the test data.
2. Plot the decision boundaries of each model together with the test data points.
3. Find the optimal Bayes classifier for this synthetic setting and compare its misclassification error on the test set to the models above.
4. Discuss how the assumptions of each model affect their performance relative to the Bayes classifier. Explore other settings such as when the ground truth class means are further apart and the effect of regularization tuning.

Derivation of the Wolfe Dual Problem

We start with the primal problem and form the Lagrangian, which incorporates the constraints using non-negative Lagrange multipliers α_i and μ_i.

$$L_P = \frac{1}{2}\|\beta\|^2 + C\sum_{i=1}^{N}\xi_i - \sum_{i=1}^{N}\alpha_i[y_i(x_i^T\beta + \beta_0) - 1 + \xi_i] - \sum_{i=1}^{N}\mu_i\xi_i$$

We minimize L_P with respect to the primal variables β, β_0, ξ_i.

$$\frac{\partial L_P}{\partial \beta} = \beta - \sum_{i=1}^{N}\alpha_i y_i x_i = 0 \quad \Longrightarrow \quad \beta = \sum_{i=1}^{N}\alpha_i y_i x_i$$

$$\frac{\partial L_P}{\partial \beta_0} = -\sum_{i=1}^{N}\alpha_i y_i = 0 \quad \Longrightarrow \quad \sum_{i=1}^{N}\alpha_i y_i = 0$$

$$\frac{\partial L_P}{\partial \xi_i} = C - \alpha_i - \mu_i = 0 \quad \Longrightarrow \quad \alpha_i = C - \mu_i$$

Substitute these conditions back into L_P. The terms involving β_0 and ξ_i cancel out, and we replace β with its expression in terms of α_i:

$$L_D = \frac{1}{2}\left\|\sum_i \alpha_i y_i x_i\right\|^2 + \cdots - \sum_i \alpha_i y_i x_i^T\left(\sum_k \alpha_k y_k x_k\right) + \sum_i \alpha_i$$

$$= \sum_{i=1}^{N}\alpha_i - \frac{1}{2}\sum_{i=1}^{N}\sum_{k=1}^{N}\alpha_i\alpha_k y_i y_k x_i^T x_k$$

The constraints $\alpha_i \geq 0$ and $\mu_i \geq 0$, combined with $\alpha_i = C - \mu_i$, imply that $0 \leq \alpha_i \leq C$. This completes the derivation of the dual problem.