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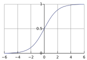
The Logistic (Sigmoid) Function

Definition

$$p(\mathbf{x}) = \sigma(t = \theta^T \mathbf{x}) = \frac{e^{\theta_0 + \theta_1 x_1}}{1 + e^{\theta_0 + \theta_1 x_1}}$$

- S-shaped (sigmoid) curve bounded between 0 and 1.
- Changes slowly at the tails and rapidly near the midpoint.
- **Numerical Example:**
  - Let $\theta_0 = -4$ and $\theta_1 = 0.02$.
  - For $x_1 = 50$: $t = -4 + 0.02 \times 50 = -3$, so

$$p(50) = \frac{e^{-3}}{1 + e^{-3}} \approx \frac{0.0498}{1.0498} \approx 0.0474.$$



  - For $x_1 = 200$: $t = -4 + 0.02 \times 200 = 0$, hence $p(200) = 0.5$.
  - For $x_1 = 300$: $t = -4 + 0.02 \times 300 = 2$, so

$$p(300) = \frac{e^2}{1 + e^2} \approx \frac{7.389}{8.389} \approx 0.88.$$

The Logit Transformation

Key Relationships

- The **logit function** is the log-odds:

$$t = \text{logit}(p) = \log\left(\frac{p}{1-p}\right)$$

- The logistic function is its inverse:

$$p = \sigma(t) = \frac{1}{1+e^{-t}}$$

- And the linear predictor is given by $t = \theta^\intercal \mathbf{x}$

Example

Numerical Example If $\widehat{p} = 0.7$, then

$$\text{log-odds} = \log\left(\frac{0.7}{0.3}\right) \approx \log(2.33) \approx 0.85.$$

Interpreting Odds and Log-Odds

Key Concepts

- **Odds:** The ratio $\frac{p(\mathbf{x})}{1-p(\mathbf{x})}$.
- **Log-Odds:**

$$\log\left(\frac{p(\mathbf{x})}{1-p(\mathbf{x})}\right) = t = \theta_0 + \theta_1 x_1$$

Example

Coefficient Interpretation If $\theta_1 = 0.5$, then for every unit increase in x_1:

- The log-odds increases by 0.5.
- The odds multiply by $e^{0.5} \approx 1.65$, meaning the odds of a positive outcome are 65% higher.

Prediction Rule: Thresholding

Threshold-based Prediction

$$\hat{y} = \begin{cases} 0 & \text{if } \widehat{p} < 0.5 \\ 1 & \text{if } \widehat{p} \geq 0.5 \end{cases}$$

- The decision boundary occurs when the linear predictor $t = \theta^\intercal \mathbf{x} = 0$.
- One predicts class 1 if the corresponding logit is nonnegative.
- The threshold (here, 0.5) can be adjusted to suit different risk tolerances.
- **Example:** If $\hat{p} = 0.3$, predict 0; if $\hat{p} = 0.8$, predict 1.

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Per-Instance Cost Function

Definition

$$c(\theta) = \begin{cases} -\log(\widehat{p}) & \text{if } y = 1 \\ -\log(1-\widehat{p}) & \text{if } y = 0 \end{cases}$$

- This cost penalizes confident but wrong predictions—cost increases steeply.
- **Example:** If $y = 1$ but $\widehat{p} = 0.1$, then cost $= -\log(0.1) \approx 2.3$.

Log Loss: Overall Cost Function

Logistic Regression Cost Function

$$J(\theta) = -\frac{1}{m}\sum_{i=1}^{m}\left[y^{(i)}\log\left(\widehat{p}^{(i)}\right) + (1 - y^{(i)})\log\left(1 - \widehat{p}^{(i)}\right)\right]$$

- This function, also known as log loss, is convex—ensuring a global minimum.
- It is derived from the maximum likelihood estimation approach.

Likelihood Function

$$\ell(\theta) = \prod_{i:y_i=1} p(x_i) \prod_{i:y_i=0} [1 - p(x_i)]$$

- Sensitive to extreme predictions; even one outlier can have a high cost.

Optimization and Gradient Descent

Gradient of the Cost Function

$$\frac{\partial J(\theta)}{\partial \theta_j} = \frac{1}{m} \sum_{i=1}^{m} \left[\sigma(\theta^\mathsf{T} \mathbf{x}^{(i)}) - y^{(i)} \right] x_j^{(i)}$$

- **Batch Gradient Descent:** Uses the entire dataset per update.
- **Stochastic Gradient Descent:** Updates parameters using a single instance.
- **Mini-batch Gradient Descent:** Uses a subset of data for each update.
- Note: Unlike linear regression, there is no closed-form solution.

Practical Training Tips

- **Feature Scaling:** Normalizing features is critical for the efficiency of gradient descent.
- **Learning Rate:** Choose carefully; consider adaptive learning rates or a line search.
- **Regularization:** To prevent overfitting, add a penalty such as:

$$\frac{\lambda}{2m}\|\theta\|^2$$

- **Convergence Monitoring:** Regularly check the cost and stop when changes become negligible.

Example: Iris dataset

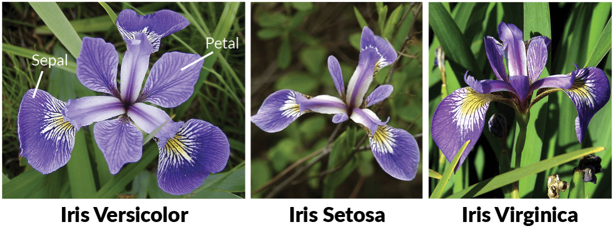


Figure: Iris Flower.

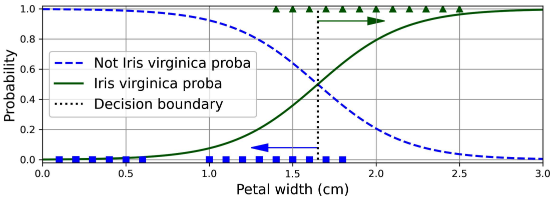


Figure: Estimated probabilities and decision boundary.

Multivariate Logistic Regression

$$\log\left(\frac{p(\mathbf{x})}{1-p(\mathbf{x})}\right) = \theta_0 + \theta_1 x_1 + \theta_2 x_2 + \cdots + \theta_p X_p$$

- Incorporates multiple predictors simultaneously.
- **Example:**
  - Univariate Model: In a study, being "Young" (e.g., under 25 years old) might show a higher car accident rate.
  - Multivariate Model: When adjusting for driving experience (e.g., years of driving), "Young" drivers might not have an inherently higher risk—their inexperience may explain the correlation.

Example: Iris dataset, Multivariate Reg.

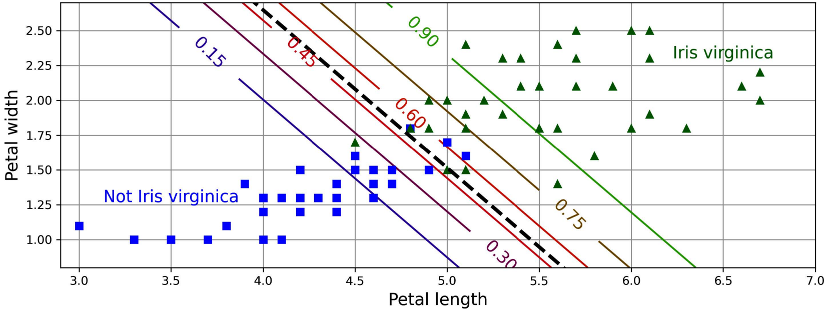


Figure: Using two features in Regression.

Multi-Class Logistic Regression

In multinomial (multi-class) logistic regression, one category is chosen as the baseline (often the K^{th} class). For each class $k \in \{1, \ldots, K-1\}$, the probability is given by:

$$\Pr(Y = k \mid X) = \frac{e^{\theta_{k0}+\theta_{k1}X_1+\cdots+\theta_{kp}X_p}}{1 + \sum_{l=1}^{K-1} e^{\theta_{l0}+\theta_{l1}X_1+\cdots+\theta_{lp}X_p}}$$

For the baseline category (class K):

$$\Pr(Y = K \mid X) = \frac{1}{1 + \sum_{l=1}^{K-1} e^{\theta_{l0}+\theta_{l1}X_1+\cdots+\theta_{lp}X_p}}$$

Multi-Class Logistic Regression

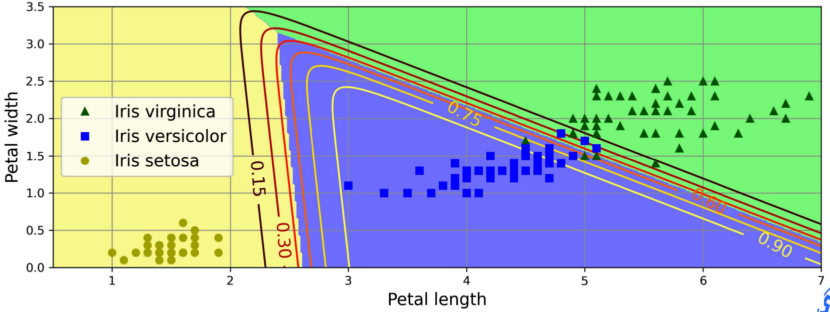
- This formulation ensures that all predicted probabilities are non-negative and sum to 1.
- While this approach models the probabilities of all classes simultaneously, an alternative is the One-vs.-Rest strategy, where separate binary classifiers are built for each class.
- Common examples include medical diagnosis (e.g., predicting whether a patient is Healthy, has a Cold, or has the Flu) and image recognition (e.g., classifying objects among several categories).
- An alternative approach is using Softmax coding as follows:

$$\Pr(Y = k \mid X) = \frac{e^{\theta_{k0} + \theta_{k1} X_1 + \cdots + \theta_{kp} X_p}}{\sum_{l=1}^{K} e^{\theta_{l0} + \theta_{l1} X_1 + \cdots + \theta_{lp} X_p}}$$

Multi-Class Logistic Regression, Example

The cost function is obtained using Cross entropy cost function:

$$J(\theta) = -\frac{1}{m}\sum_{i=1}^{m}\sum_{k=1}^{K}\left[y_k^{(i)}\log\left(\widehat{p}_k^{(i)}\right)\right]$$



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Assumptions and Limitations

- **Linear Decision Boundary:**
  - Assumes that the log-odds of the outcome are a *linear combination* of the predictors.
  - This means any non-linear relationship must be handled through transformations or additional terms.
- **Feature Independence:**
  - Predictors should have minimal multicollinearity.
  - High correlation between features can lead to unstable and unreliable estimates.
- **Distribution of Errors:**
  - Implicitly assumes that the error distribution is roughly logistic.
  - Deviations from this assumption might affect model performance.
- **Sample Size:**
  - A general guideline is to have about 10 events (i.e., occurrences of the less frequent outcome) per predictor.
  - This helps ensure stable and reliable parameter estimates.

Conclusion and Key Takeaways

When to Use Logistic Regression

- Baseline Model: Ideal for binary and categorical classification tasks due to its simplicity.
- Interpretability: Provides clear, interpretable estimates of feature importance through odds ratios.
- Probability Estimates: Outputs well-calibrated probabilities, useful for decision-making processes.

- Logistic Regression is robust and interpretable for classification tasks.
- Its foundation in probability theory (MLE) makes it statistically sound.
- Understanding the transformation from linear predictors to probabilities (via the logistic function) is key.
- Practical considerations—feature scaling, regularization, and optimization—can significantly enhance model performance.

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Motivation — An Alternative Approach

- Traditional approaches (like Logistic Regression) directly model the conditional probability $\Pr(Y \mid X)$.
- LDA adopts a generative approach that models $\Pr(X \mid Y)$ and then uses Bayes' theorem:
- This formulation can be more efficient when class-conditional densities $(Pr(X|Y = k))$ are Gaussian and the sample size is small.

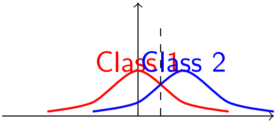


Figure: Visualization of Gaussian class densities and decision boundary

Comparison: Logistic Regression vs. LDA

Logistic Regression

- Direct probability modeling: $\Pr(Y \mid X)$
- No explicit distributional assumptions
- Tends to be more stable when there are many predictors

LDA

- Assumes Gaussian class-conditional densities
- Naturally extends to multi-class problems
- Often more efficient when sample size is small

Example: For 3 classes with 10 samples per class, the parametric form of LDA can be advantageous compared to the flexibility (and potential overfitting) of logistic regression.

Bayes' Theorem & Classifier

Bayes' Rule for Classification:

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

- π_k: Prior probability of class k $\rightarrow \Pr(Y=k)$
- $f_k(x)$: Class-conditional density of X for $Y = k$ $\rightarrow \Pr(X=x | Y=k)$
- Decision Rule: Assign x to class k maximizing $\Pr(Y = k | X = x)$

Bayes Error Rate: Minimum possible error rate if true densities $f_k(x)$ are known.

Challenge: Estimating $f_k(x)$ from data.

Assume class densities are multivariate Gaussian with **shared covariance**:

$$f_k(x) = \frac{1}{(2\pi)^{p/2}|\Sigma|^{1/2}} \exp\left(-\frac{1}{2}(x-\mu_k)^T\Sigma^{-1}(x-\mu_k)\right)$$

Key Implications:

- Linear decision boundaries
- Homoscedasticity: Same covariance structure across classes

$$\pi_k f_k(x) = \pi_k \cdot \frac{1}{\sqrt{2\pi}\sigma} \exp\left[\frac{-(x-\mu_k)^2}{2\sigma^2}\right] \rightarrow \frac{-(x^2+\mu_k^2-2x\mu_k)}{2\sigma^2}$$

$$\log \rightarrow \quad \log \pi_k - \frac{x^2}{2\sigma^2} - \frac{\mu_k^2}{2\sigma^2} + x\mu_k/\sigma^2$$

Derivation of LDA Discriminant Function

Starting from Bayes' rule, take log and simplify:

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

- Quadratic terms cancel due to shared Σ
- Decision boundary between classes k and l: $\delta_k(x) = \delta_l(x)$

For $p = 1$ **(Simplified)**:

$$\delta_k(x) = \frac{\mu_k}{\sigma^2} x - \frac{\mu_k^2}{2\sigma^2} + \log \pi_k$$

Boundary: $x = \frac{\mu_1 + \mu_2}{2}$ when $\pi_1 = \pi_2$

Graphical Illustration — 1D Case

- **Left:** Two Gaussian densities $f_1(x)$ and $f_2(x)$
- **Dashed line:** Bayes decision boundary

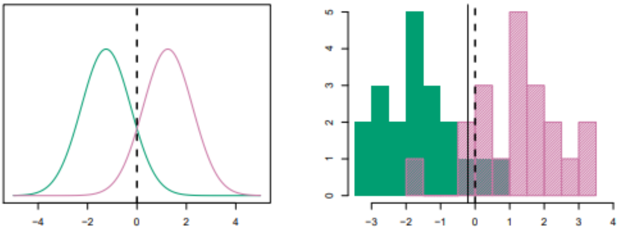


Figure: 1D Gaussian densities and decision boundary.

Parameter Estimation in LDA

Maximum Likelihood Estimators:

- Class mean:

$$\hat{\mu}_k = \frac{1}{n_k} \sum_{i:y_i=k} x_i$$

- Pooled covariance:

$$\hat{\Sigma} = \frac{1}{n-K} \sum_{k=1}^{K} \sum_{i:y_i=k} (x_i - \hat{\mu}_k)(x_i - \hat{\mu}_k)^T$$

- Prior probabilities:

$$\hat{\pi}_k = \frac{n_k}{n}$$

Intuition: $\hat{\Sigma}$ is a weighted average of class-specific covariances.

Example: LDA for $p = 1$ with Calculations

Simulated Data:

- Class 1: $\mu_1 = -1.25$, Class 2: $\mu_2 = 1.25$, $\sigma^2 = 1$
- Training data: $n_1 = n_2 = 20$

Estimates:

$$\hat{\mu}_1 = -1.2,\ \hat{\mu}_2 = 1.3,\ \hat{\sigma}^2 = 0.95$$

Decision Boundary:

$$x = \frac{\hat{\mu}_1 + \hat{\mu}_2}{2} = \frac{-1.2 + 1.3}{2} = 0.05$$

- Bayes boundary: $x = 0$ (vs. LDA: $x = 0.05$)
- Error rates: Bayes (10.6%), LDA (11.1%)

Case Study: Default Data Analysis

Confusion Matrix (Threshold=0.5):

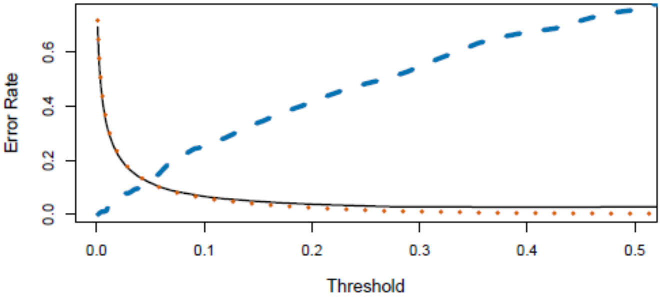
		True No	True Yes	Total
Predicted	**No**	9644 (TN)	252 (FN)	9896
	Yes	23 (FP)	81 (TP)	104
	Total	9667	333	10000

Confusion Matrix (Threshold=0.2):

		True No	True Yes	Total
Predicted	**No**	9432 (TN)	138 (FN)	9570
	Yes	235 (FP)	195 (TP)	430
	Total	9667	333	10000

Threshold Tuning

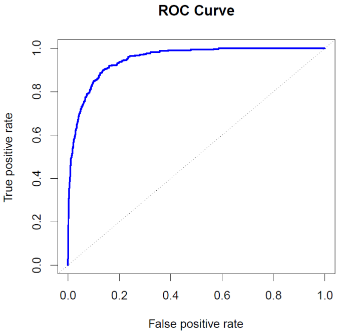
- The black solid line displays the overall error rate.
- The blue dashed line represents the fraction of defaulting customers that are incorrectly classified,
- The orange dotted line indicates the fraction of errors among the non-defaulting customers.



Threshold Tuning & ROC Curve

Adjusting Posterior Threshold:

- Lower threshold (e.g., 0.2) increases sensitivity (TP/P) but decreases specificity ($FP/N = 1-$specificity)
- Trade-off captured by ROC curve



ROC curve: AUC $= 0.95$ (Excellent discrimination)

Graphical Illustration — Multivariate LDA

- **Left:** Three-class example with 95% probability ellipses
- **Dashed lines:** Bayes decision boundaries
- **Solid lines:** LDA estimated boundaries

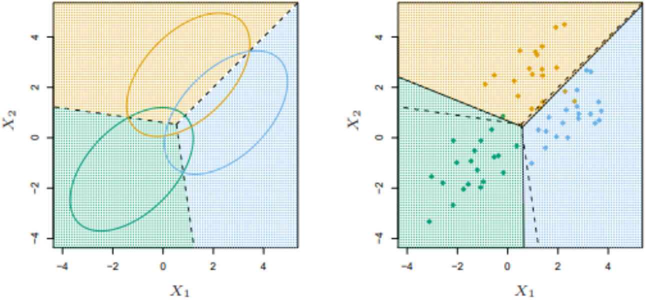


Figure: Multivariate LDA: Bayes vs. LDA boundaries.

QDA: Model Assumptions

Relax LDA's assumption: Class-specific covariances:

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

Discriminant Function:

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

- Quadratic terms in x remain $\Rightarrow$ Quadratic boundaries

LDA vs. QDA: Mathematical Comparison

	LDA	**QDA**
Covariance	Shared (Σ)	Class-specific (Σ_k)
Discriminant	Linear in x	Quadratic in x
Parameters	$Kp + \frac{p(p+1)}{2}$	$K\left(p + \frac{p(p+1)}{2}\right)$
Bias-Variance	Low variance, high bias*	High variance, low bias*

*When assumptions are violated.

Example: For $p = 2$, $K = 2$: LDA (7 parameters), QDA (11 parameters)

When to Use LDA vs. QDA?

- **LDA preferred**:
  - Small sample size ($n < 5p$)
  - Shared covariance structure (e.g., similar class spreads)
  - High-dimensional data (regularization needed)
- **QDA preferred**:
  - Large sample size ($n > 10p$)
  - Heteroscedastic classes (unequal covariances)
  - Complex decision boundaries

Summary

- **LDA**: Efficient, linear boundaries, requires $n > p$
- **QDA**: Flexible, quadratic boundaries, needs larger n
- Model choice depends on bias-variance trade-off and data structure
- Threshold tuning critical for imbalanced class problems
- Always validate assumptions and consider alternatives

LDA and QDA

- Left: The Bayes (purple dashed), LDA (black dotted), and QDA (green solid) decision boundaries for a two-class problem. $\Sigma_1 = \Sigma_2$. The shading indicates the QDA decision rule. Since the Bayes decision boundary is linear, it is more accurately approximated by LDA than by QDA.
- Right: Details are as given in the left-hand panel, except that $\Sigma_1 \neq \Sigma_2$