Introduction to Machine Learning CS182

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Feb. 28, 2023

Today:

- Linear Methods for Classification II
 - Generalization of LDA
 - Logistic Regression
 - Summary

Readings:

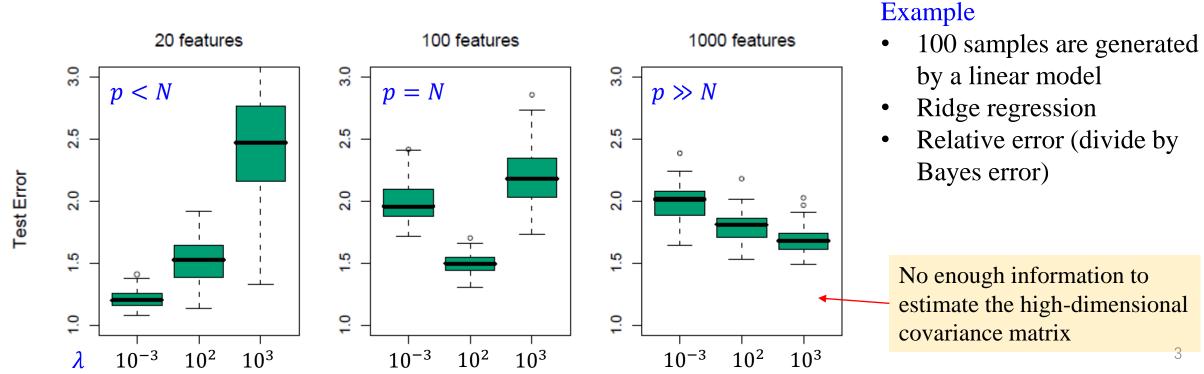
• The Elements of Statistical Learning (ESL), Chapters 4.3, 4.4, 18.1, 18.2 and 18.3

Linear Methods for Classification II

- Generalization of LDA
 - Regularized Discriminant Analysis
 - Fisher's Formulation of Discriminant Analysis
- Logistic Regression
- Summary

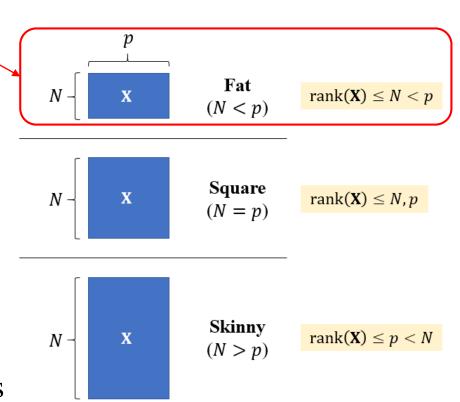
High dimensional problems $(p \gg N)$

- genomics problem, signal/image analysis
- Less fitting is better



High dimensional problems $(p \gg N)$

- Cannot fit LDA to the data
 - \Box inversion of a $p \times p$ covariance matrix Σ
 - \square Σ is singular, due to rank(Σ) $\leq N \ll p$
- Regularization is necessary
 - No enough data to estimate feature dependencies
 - E.g., independent assumption on features
 - > Diagonal within-class covariance matrix #paras: $K \times p \times p \rightarrow K \times p$



Regularized LDA (RLDA)

• Shrinks $\hat{\Sigma}$ towards its diagonal

$$\hat{\Sigma}(\gamma) = \gamma \hat{\Sigma} + (1 - \gamma) \operatorname{diag}(\hat{\Sigma}), \gamma \in [0, 1]$$

where diag($\hat{\Sigma}$) denotes a diagonal matrix sharing the same diagonal elements with $\hat{\Sigma}$

Diagonal LDA

• Independent assumption on feature dependencies

$$\hat{\Sigma} = \operatorname{diag}(\hat{\Sigma})$$

A brief summary of generalized LDA ($\alpha, \gamma \in [0, 1]$)

	Method	Covariance matrix	Effect
Linear	Regularized LDA (RLDA)	$\widehat{\Sigma}(\gamma) = \gamma \widehat{\Sigma} + (1 - \gamma) \operatorname{diag}(\widehat{\Sigma})$	Shrink $\widehat{\Sigma}$ towards diag($\widehat{\Sigma}$)
	Diagonal LDA	$\widehat{\Sigma} = \operatorname{diag}(\widehat{\Sigma})$	Make features independent
Quadratic	Regularized QDA (RQDA)	$\widehat{\mathbf{\Sigma}}_k(\alpha) = \alpha \widehat{\mathbf{\Sigma}}_k + (1 - \alpha) \widehat{\mathbf{\Sigma}}$	Shrink $\widehat{\Sigma}_k$ towards $\widehat{\Sigma}$ (LDA + QDA)
	Variant of RQDA	$\widehat{\Sigma}_k(\alpha, \gamma) = \alpha \widehat{\Sigma}_k + (1 - \alpha) \widehat{\Sigma}(\gamma)$	Shrink $\widehat{\Sigma}_k$ towards $\widehat{\Sigma}(\gamma)$ (RLDA + QDA)

Regularized Discriminant Analysis on the Vowel Data

https://hastie.su.domains/ElemStatLearn/

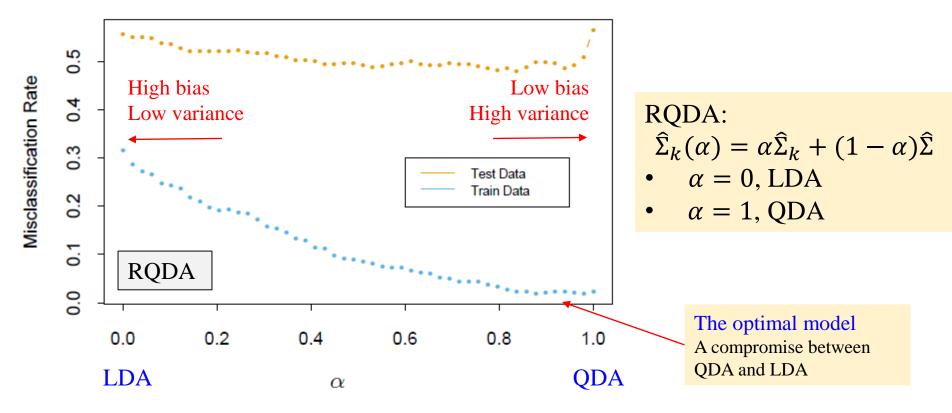
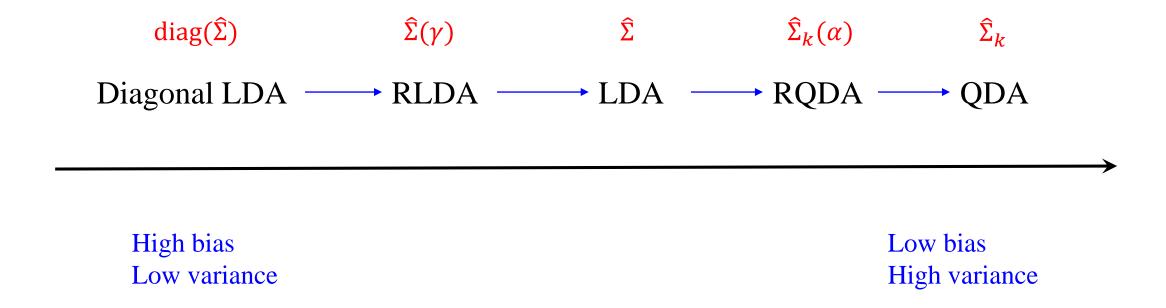


FIGURE 4.7. Test and training errors for the vowel data, using regularized discriminant analysis with a series of values of $\alpha \in [0, 1]$. The optimum for the test data occurs around $\alpha = 0.9$, close to quadratic discriminant analysis.



LDA: Approach 1

- 1. Estimating $\hat{\Sigma}$, $\hat{\mu}_k$ and $\hat{\pi}_k$
- 2. Discriminant function

$$\delta_k(x) = x^T \widehat{\mathbf{\Sigma}}^{-1} \widehat{\mu}_k - \frac{1}{2} \widehat{\mu}_k^T \widehat{\mathbf{\Sigma}}^{-1} \widehat{\mu}_k + \log \widehat{\pi}_k$$

3. Classify to class *k* that maximizes the discriminant function

$$\widehat{G}(x) = \operatorname*{argmax}_{k \in \mathcal{G}} \delta_k(x)$$

LDA: Approach 2

- 1. Estimating $\widehat{\Sigma}$, $\hat{\mu}_k$ and $\hat{\pi}_k$
- 2. Eigen-decomposition:

$$\widehat{\mathbf{\Sigma}} = \mathbf{U}\mathbf{D}\mathbf{U}^T$$

3. Data sphering $(\hat{\Sigma}^* = \mathbf{I})$

$$\mathbf{x}^* = \mathbf{D}^{-\frac{1}{2}} \mathbf{U}^T \mathbf{x} = \widehat{\mathbf{\Sigma}}^{-\frac{1}{2}} \mathbf{x}$$

$$\hat{\mu}_{\nu}^* = \mathbf{D}^{-\frac{1}{2}} \mathbf{U}^T \hat{\mu}_{\nu} = \widehat{\mathbf{\Sigma}}^{-\frac{1}{2}} \hat{\mu}_{\nu}$$

4. Classify to its closest class centroid in the transformed space $\widehat{G}(x) = \operatorname{argmin} \frac{1}{2} \|x^* - \widehat{\mu}_k^*\|^2 - \ln \widehat{\pi}_k$

1.
$$\log \frac{\Pr(G=k|X=x)}{\Pr(G=\ell|X=x)} = \delta_k(x) - \delta_\ell(x)$$

2. $\delta_k(x) \propto \log \Pr(G=k|X=x)$

Pr(G=k|X=x) = $\frac{\Pr(X=x|G=k)\Pr(G=k)}{\Pr(X=x)}$

3. $\log \Pr(G=k|X=x) = -\frac{1}{2}(x-\hat{\mu}_k)^T \widehat{\Sigma}^{-1}(x-\hat{\mu}_k) + \log \widehat{\pi}_k + C$

Constant

3.
$$\log \Pr(G = k | X = x) = -\frac{1}{2} (x - \hat{\mu}_k)^T \widehat{\Sigma}^{-1} (x - \hat{\mu}_k) + \log \widehat{\pi}_k + C$$
 Constant
$$= -\frac{1}{2} (x - \hat{\mu}_k)^T \mathbf{U} \mathbf{D}^{-\frac{1}{2}} (\mathbf{U} \mathbf{D}^{-\frac{1}{2}})^T (x - \hat{\mu}_k) + \log \widehat{\pi}_k + C$$

$$= -\frac{1}{2} (\mathbf{D}^{-\frac{1}{2}} \mathbf{U}^T x - \mathbf{D}^{-\frac{1}{2}} \mathbf{U}^T \hat{\mu}_k)^T (\mathbf{D}^{-\frac{1}{2}} \mathbf{U}^T x - \mathbf{D}^{-\frac{1}{2}} \mathbf{U}^T \hat{\mu}_k) + \log \widehat{\pi}_k + C$$

$$= -\frac{1}{2} (x^* - \hat{\mu}_k^*)^T (x^* - \hat{\mu}_k^*) + \log \widehat{\pi}_k + C$$

$$= -\frac{1}{2} ||x^* - \hat{\mu}_k^*||^2 + \ln \widehat{\pi}_k + C$$

4.
$$\hat{G}(x) = \underset{k \in \mathcal{G}}{\operatorname{argmax}} \, \delta_k(x) = \underset{k \in \mathcal{G}}{\operatorname{argmax}} \log \Pr(G = k | X = x) = \underset{k \in \mathcal{G}}{\operatorname{argmin}} \frac{1}{2} \|x^* - \hat{\mu}_k^*\|^2 - \ln \hat{\pi}_k$$

LDA: Approach 1

- 1. Estimating $\widehat{\Sigma}$, $\widehat{\mu}_k$ and $\widehat{\pi}_k$ Complexity $\mathcal{O}(p^3)$
- 2. Discriminant function $\delta_k(x) = x^T \widehat{\Sigma}^{-1} \widehat{\mu}_k \frac{1}{2} \widehat{\mu}_k^T \widehat{\Sigma}^{-1} \widehat{\mu}_k + \log \widehat{\pi}_k$
- 3. Classify to class k that maximizes the discriminant function $\widehat{G}(x) = \operatorname*{argmax}_{k \in G} \delta_k(x)$
- Two approaches have almost the same time and storage complexity
- Approach 2 shows the potential of LDA for dimension reduction

LDA: Approach 2

- 1. Estimating $\widehat{\Sigma}$, $\hat{\mu}_k$ and $\hat{\pi}_k$
- 2. Eigen-decomposition:

$$\widehat{\Sigma} = \mathbf{U}\mathbf{D}\mathbf{U}^T$$

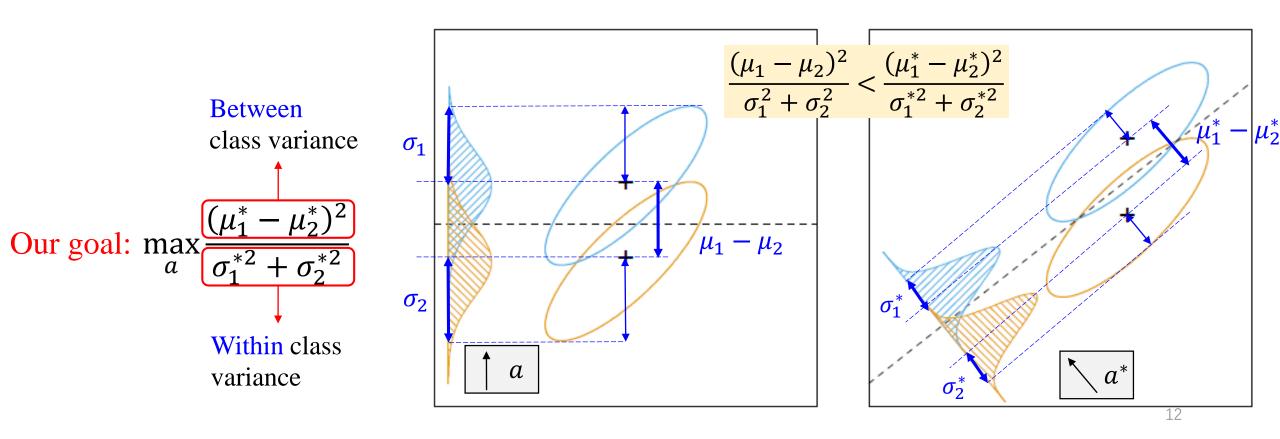
3. Data sphering $(\hat{\Sigma}^* = \mathbf{I})$

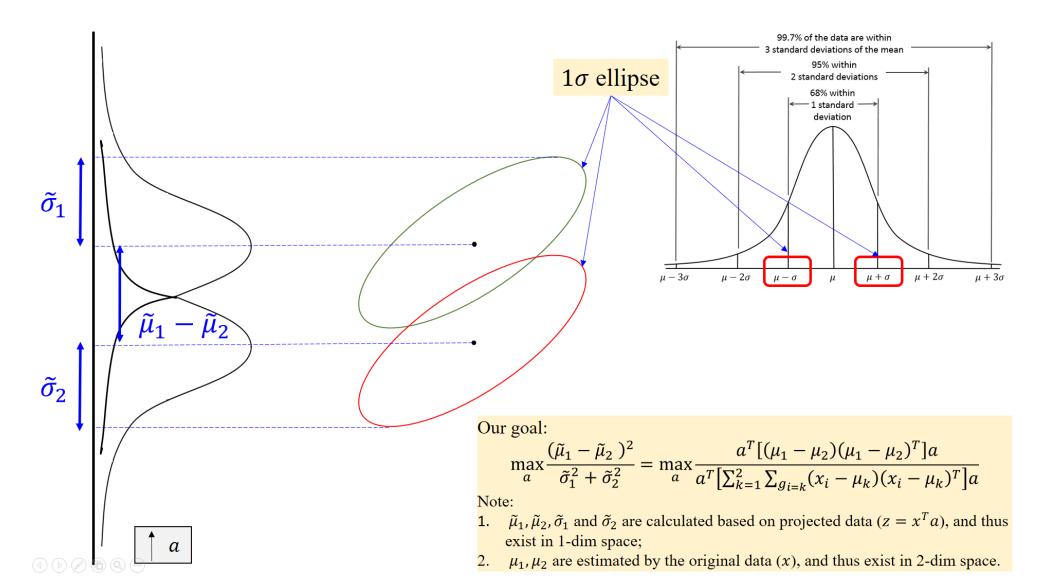
$$\mathbf{x}^* = \mathbf{D}^{-\frac{1}{2}} \mathbf{U}^T \mathbf{x} = \widehat{\mathbf{\Sigma}}^{-\frac{1}{2}} \mathbf{x}$$

$$\hat{\mu}_{\nu}^* = \mathbf{D}^{-\frac{1}{2}} \mathbf{U}^T \hat{\mu}_{\nu} = \widehat{\mathbf{\Sigma}}^{-\frac{1}{2}} \hat{\mu}_{\nu}$$

4. Classify to its closest class centroid in the transformed space $\widehat{G}(x) = \underset{k \in \mathcal{G}}{\operatorname{argmin}} \frac{1}{2} \|x^* - \widehat{\mu}_k^*\|^2 - \ln \widehat{\pi}_k$

• Find $z = x^T a$ such that the between class variance is maximized relative to the within class variance.





Maximize the Rayleigh quotient:

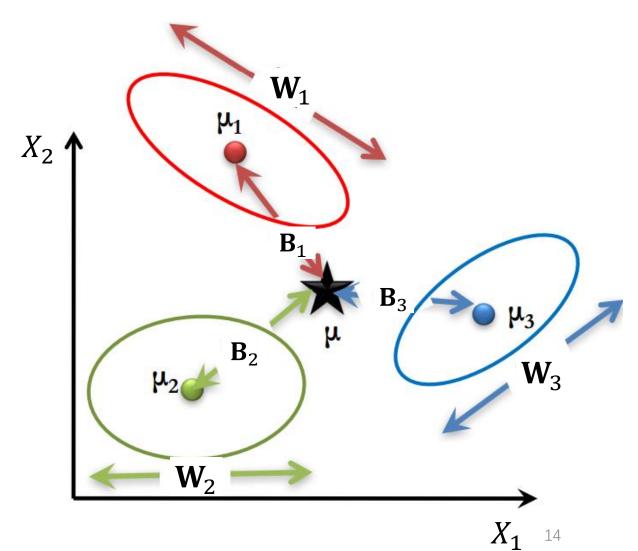
$$\max_{a} \frac{a^T \mathbf{B} a}{a^T \mathbf{W} a}$$

Between class variance

$$\mathbf{B} = \sum_{k=1}^{K} N_k (\mu_k - \bar{\mu}) (\mu_k - \bar{\mu})^T$$

Within class variance

$$\mathbf{W} = \sum_{k=1}^{K} \sum_{g_i = k} (x_i - \bar{\mu}_k) (x_i - \bar{\mu}_k)^T$$



• Maximize the Rayleigh quotient:

$$\max_{a} \frac{a^T \mathbf{B} a}{a^T \mathbf{W} a}$$

Between class variance

$$\mathbf{B} = \sum_{k=1}^{K} N_k (\mu_k - \bar{\mu}) (\mu_k - \bar{\mu})^T$$

Within class variance

$$\mathbf{W} = \sum_{k=1}^{K} \sum_{g_i = k} (x_i - \bar{\mu}_k) (x_i - \bar{\mu}_k)^T$$

• Equivalently,

$$\max_{a} a^{T} \mathbf{B} a$$

$$s.t. a^{T} \mathbf{W} a = 1$$

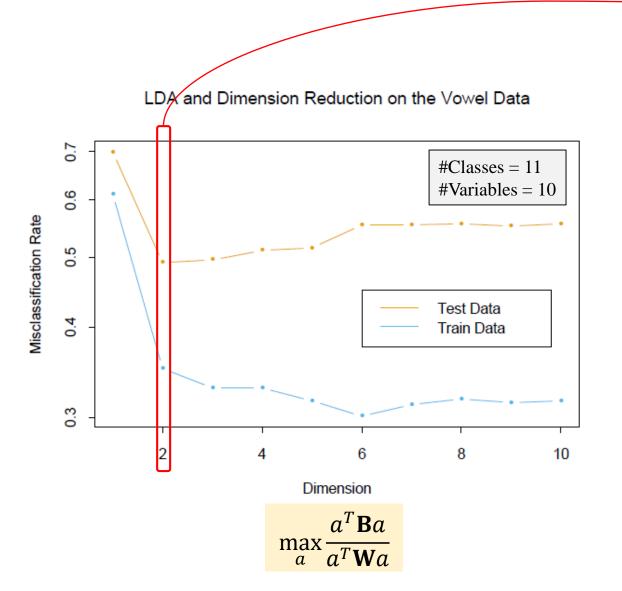
- a is discriminant coordinates (canonical variates)
- Generalized eigenvalue problem $\mathbf{B}a = \lambda \mathbf{W}a$

which can be efficiently solved

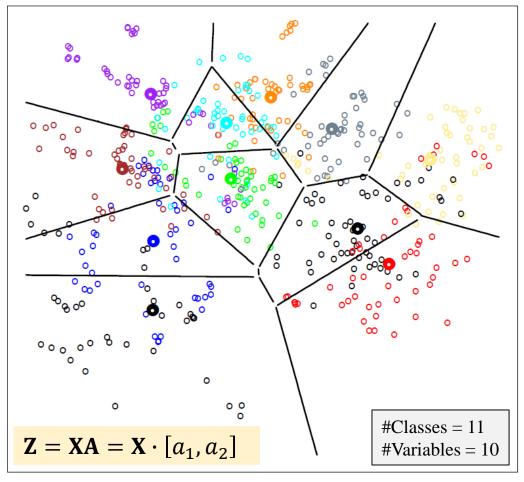
Ex. 4.1.

Hint: Lagrangian multipliers

Canonical Coordinate 2



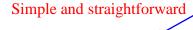
Classification in Reduced Subspace



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Classification



Linear regression

$$\mathcal{G} = \{1, 2 \dots, K\}$$

Indicator matrix
$$\mathbf{Y} = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}$$

Multi-output regression

Prediction
$$\hat{f}(x) = \hat{\mathbf{B}}^T \begin{pmatrix} 1 \\ x \end{pmatrix} = \begin{pmatrix} \hat{f}_1(x) \\ \hat{f}_2(x) \\ \vdots \\ \hat{f}_K(x) \end{pmatrix}$$

$$\hat{G}(x) = \underset{k \in \mathcal{G}}{\operatorname{argmax}} \hat{f}_k(x)$$

Limitation

The masking problem $(K \ge 3)$

min_fEPE

Theoretical

Squared error loss

 $f(x) = \mathrm{E}(Y|X=x)$

Least squares

Linear

Nearest neighbors

Nonlinear

Regression

Bayes classifier

Zero-one loss

$$\widehat{G}(x) = \underset{k \in \mathcal{G}}{\operatorname{argmax}} \Pr(G = k | X = x)$$

$$(0,1) \rightarrow (-\infty, +\infty)$$

Logit transformation $\log t(x) = \log \left(\frac{x}{1-x}\right)$

Pairwise odds = 1

Decision boundary $\log \frac{\Pr(G = k | X = x)}{\Pr(G = \ell | X = x)} = 0$

Can we **directly model** the decision boundary?

$$\Pr(G = k | X = x)$$

$$= \frac{\Pr(X = x | G = k) \Pr(G = k)}{\Pr(X = x)}$$

$$\text{LDA, QDA,}$$

$$\text{RDA}$$

Logistic regression₈

Linear Discriminant Analysis

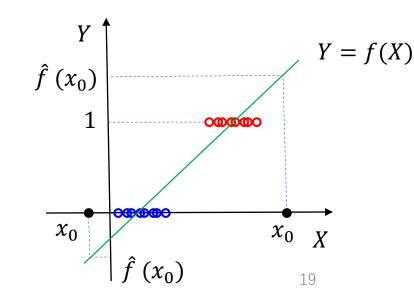
• Recall our discussion on linear regression of an indicator matrix

Linear classification: Minimizing EPE:
$$\widehat{G}(x) = \operatorname*{argmax} \widehat{f}_k(x)$$

$$\widehat{G}(x) = \operatorname*{argmax} \Pr(G = k | X = x)$$

$$k \in \mathcal{G}$$

- It is inappropriate to represent a posterior directly by a linear function.
- Solution: make some monotone transformation of the posterior be linear in *X*



Linear decision boundary

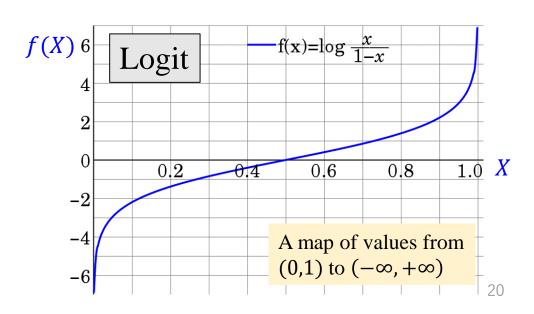
Linear Discriminant Analysis

• Logit transform

$$logit(Pr(x)) = log\left(\frac{Pr(x)}{1 - Pr(x)}\right)$$

It maps $Pr(x) \in (0,1)$ to $logit(Pr(x)) \in (-\infty, +\infty)$

- Decision boundary
 - Odds equals to 1
 - Or, logit equals to 0



Odds (发生比)

Linear Discriminant Analysis

• Example: binary (two class) classification

Logit:
$$\log \frac{\Pr(G=1|X=x)}{1-\Pr(G=1|X=x)} = \log \frac{\Pr(G=1|X=x)}{\Pr(G=2|X=x)} = \beta_0 + x^T \beta$$

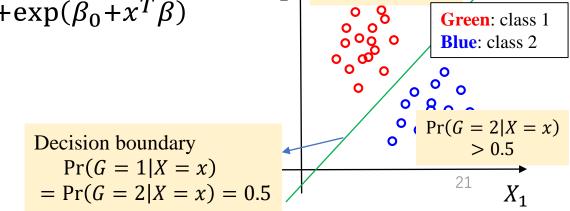
• The posterior probability

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

$$Pr(G = 2|X = x) = \frac{1}{1 + \exp(\beta_0 + x^T \beta)}, X_2 \uparrow \begin{cases} \Pr(G = 1|X = x) \\ > 0.5 \end{cases}$$

• Decision boundary

$$\{x|\beta_0 + x^T\beta = 0\}$$



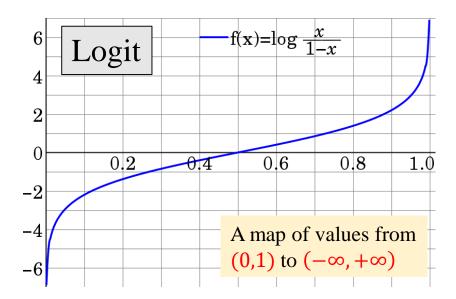
• Model the posterior probabilities of the *K* classes via linear function in *x*.

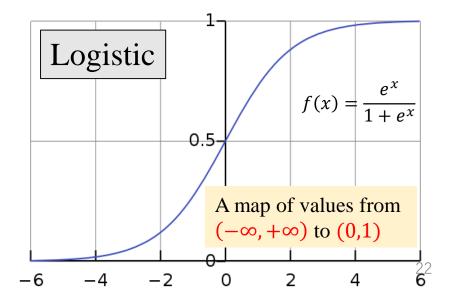
$$\log \frac{\Pr(G = 1|X = x)}{\Pr(G = K|X = x)} = \beta_{10} + x^T \beta_1$$
$$\log \frac{\Pr(G = 2|X = x)}{\Pr(G = K|X = x)} = \beta_{20} + x^T \beta_2$$
$$\vdots$$

$$\log \frac{\Pr(G = K - 1 | X = x)}{\Pr(G = K | X = x)} = \beta_{(K-1)0} + x^T \beta_{K-1}$$

• K - 1 log-odds or logit function $Pr(x) = \log \frac{Pr(x)}{1 - Pr(x)}$

• The inverse of logit is logistic function





• Model the posterior probabilities of the *K* classes via linear function in *x*.

$$\log \frac{\Pr(G = 1|X = x)}{\Pr(G = K|X = x)} = \beta_{10} + x^T \beta_1$$

$$\log \frac{\Pr(G = 2|X = x)}{\Pr(G = K|X = x)} = \beta_{20} + x^T \beta_2$$
:

$$\log \frac{\Pr(G = K - 1 | X = x)}{\Pr(G = K | X = x)} = \beta_{(K-1)0} + x^T \beta_{K-1}$$

• K - 1 log-odds or logit function $Pr(x) = \log \frac{Pr(x)}{1 - Pr(x)}$

• The inverse of logit is logistic function

• A simple calculation yields

$$\Pr(G = k | X = x) = \frac{\exp(\beta_{k0} + x^T \beta_k)}{1 + \sum_{\ell=1}^{K-1} \exp(\beta_{\ell0} + x^T \beta_\ell)},$$

$$k = 1, ..., K - 1$$

$$\Pr(G = K | X = x) = \frac{1}{1 + \sum_{\ell=1}^{K-1} \exp(\beta_{\ell0} + x^T \beta_\ell)}$$

Parameter set

$$\theta = \{\beta_{10}, \beta_1, \dots, \beta_{(K-1)0}, \beta_{K-1}\}$$

• #parameters = $(p + 1) \times (K - 1)$

$$\log \frac{\Pr(G = 1 | X = x)}{\Pr(G = K | X = x)} = \beta_{10} + x^{T} \beta_{1}$$

$$\vdots$$

$$\log \frac{\Pr(G = K - 1 | X = x)}{\Pr(G = K | X = x)} = \beta_{(K-1)0} + x^{T} \beta_{K-1}$$

$$\sum_{\ell=1}^{K-1} \Pr(G = \ell | X = x) = \Pr(G = K | X = x) \exp(\beta_{10} + x^{T} \beta_{1})$$

$$\vdots$$

$$\Pr(G = K - 1 | X = x) = \Pr(G = K | X = x) \exp(\beta_{(K-1)0} + x^{T} \beta_{K-1})$$

$$\sum_{\ell=1}^{K-1} \Pr(G = \ell | X = x) = 1 - \Pr(G = K | X = x)$$

$$\Pr(G = K | X = x) = \frac{\sum_{\ell=1}^{K-1} \exp(\beta_{\ell 0} + x^{T} \beta_{\ell})}{1 + \sum_{\ell=1}^{K-1} \exp(\beta_{\ell 0} + x^{T} \beta_{\ell})}, k = 1, ..., K - 1$$

$$24$$

- Estimating parameter set $\theta = \{\beta_{10}, \beta_1, ..., \beta_{(K-1)0}, \beta_{K-1}\}$ Maximum likelihood estimation (MLE)
- Log-likelihood for *N* observations

$$\ell(\theta) = \log \Pr(\mathbf{g}|\mathbf{X}; \theta) = \sum_{i=1}^{N} \log \Pr(g_i|x_i; \theta)$$

- Two classes
 - Bernoulli distribution

$$\Pr(g = y | x; \theta) = p(x; \theta)^{y} (1 - p(x; \theta))^{1-y}$$

Class	g = 1	g=2
Code	y = 1	y = 0
Probability	$p(x;\theta)$	$1 - p(x; \theta)$

• Two classes
$$p(x;\theta) = \Pr(G = 1|X = x;\theta) = \frac{\exp(\beta_0 + x^T \beta)}{1 + \exp(\beta_0 + x^T \beta)}$$

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

$$= \sum_{i=1}^{N} \{ y_i \left[x^T \beta - \log\left(1 + e^{x_i^T \beta}\right) \right] - (1 - y_i) \log\left(1 + e^{x_i^T \beta}\right) \}$$

$$= \sum_{i=1}^{N} \{ y_i x_i^T \beta - \log\left(1 + e^{x_i^T \beta}\right) \} \leftarrow \frac{x_i \leftarrow \begin{pmatrix} 1 \\ x_i \end{pmatrix}}{\beta \leftarrow \begin{pmatrix} \beta_0 \\ \beta \end{pmatrix}}$$

• The *first* derivative of $\ell(\theta)$

$$\frac{\partial \ell(\beta)}{\partial \beta} = \sum_{i=1}^{N} \left(y_i x_i - \frac{\exp(x^T \beta)}{1 + \exp(x^T \beta)} \right)$$
$$= \sum_{i=1}^{N} x_i (y_i - p(x_i))$$

• The *second* derivative (Hessian)

$$\frac{\partial^2 \ell(\beta)}{\partial \beta \partial \beta^T} = \sum_{i=1}^N -x_i \left(\frac{\partial p(x_i)}{\partial \beta^T} \right) = -\sum_{i=1}^N x_i x_i^T p(x_i) (1 - p(x_i))$$

 β^{old}

In matrix form

$$\frac{\partial \ell(\beta)}{\partial \beta} = \mathbf{X}^T (\mathbf{y} - \mathbf{p})$$
$$\frac{\partial^2 \ell(\beta)}{\partial \beta \partial \beta^T} = -\mathbf{X}^T \mathbf{W} \mathbf{X}$$

where $\mathbf{W} \in \mathbb{R}^{N \times N}$ is a diagonal matrix with the *i*-th diagonal element $p(x_i)(1-p(x_i))$

The Newton-Raphson algorithm: find the minimum or maximum iteratively by

$$x^{\text{new}} = x^{\text{old}} - \frac{f'(x^{\text{old}})}{f''(x^{\text{old}})}$$

• The Newton-Raphson step:

$$\beta^{\text{new}} = \beta^{\text{old}} - \left(\frac{\partial^{2}\ell(\beta)}{\partial\beta\partial\beta^{T}}\right)^{-1} \frac{\partial\ell(\beta)}{\partial\beta}$$

$$= \beta^{\text{old}} + (\mathbf{X}^{T}\mathbf{W}\mathbf{X})^{-1}\mathbf{X}^{T}(\mathbf{y} - \mathbf{p})$$

$$= (\mathbf{X}^{T}\mathbf{W}\mathbf{X})^{-1}\mathbf{X}^{T}\mathbf{W}(\mathbf{X}\beta^{\text{old}} + \mathbf{W}^{-1}(\mathbf{y} - \mathbf{p}))$$

$$= (\mathbf{X}^{T}\mathbf{W}\mathbf{X})^{-1}\mathbf{X}^{T}\mathbf{W}\mathbf{z}$$

• Given the response

$$z = X\beta^{\text{old}} + W^{-1}(y - p),$$

• it is represented as a weighted least squares problem:

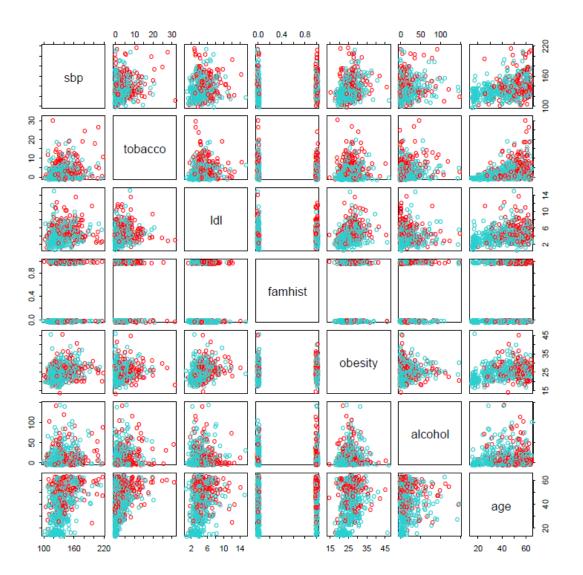
$$\beta^{\text{new}} \leftarrow \operatorname{argmin}_{\beta} (\mathbf{z} - \mathbf{X}\beta)^T \mathbf{W} (\mathbf{z} - \mathbf{X}\beta)$$

• Iteratively reweighted least squares (IRLS) algorithm

- Initialize β
- 2. Repeat3. Form linearized responses

$$z_i = x_i^T \beta + \frac{y_i - p_i}{p_i (1 - p_i)} \leftarrow \mathbf{z} = \mathbf{X} \beta^{\text{old}} + \mathbf{W}^{-1} (\mathbf{y} - \mathbf{p})$$

- 4. Form weights w_i = p_i(1 p_i)
 5. Update β by weighted least squares of z_i on x_i with w_i, ∀i
 6. Until convergence β^{new} ← argmin_β(z Xβ)^TW(z Xβ)



Example: South African Heart Disease

• Red: 160 cases

• Green: 302 controls

• Z score measures the significance of a coefficient

	Coefficient	Std. Error	Z Score	
sbp	0.006	0.006	1.023	收缩压
tobacco	0.080	0.026	3.034	
ldl	0.185	0.057	3.219	
famhist	0.939	0.225	4.178	
obesity	-0.035	0.029	-1.187	肥胖
alcohol	0.001	0.004	0.136	饮酒
age	0.043	0.010	4.184	

The data is fitted by logistic regression

• L₁ regularized logistic regression

$$\max_{\beta_0,\beta} \left\{ \sum_{i=1}^{N} \left[y_i (\beta_0 + \beta^T x_i) - \log(1 + e^{\beta_0 + \beta^T x_i}) \right] - \lambda \sum_{j=1}^{p} |\beta_j| \right\}$$

- Standardize the inputs, and penalize without β_0
- Solved by the Newton algorithm
 - Replace the weighted least squares by the weighted lasso.
- L_2 regularized logistic regression? Algorithm?

Connection between LDA and Logistic Regression

- The linear logistic model only specifies the conditional distribution, while the LDA model specifies the joint distribution
- If the additional assumption made by LDA is appropriate, LDA tends to estimate the parameters more efficiently.
- Another advantage of LDA is that samples without class labels can be used under the model of LDA. On the other hand, LDA is not robust to gross outliers. Because logistic regression relies on fewer assumptions, it seems to be more robust to the non-Gaussian type of data.
- In practice, logistic regression and LDA often give similar results.

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