Optimization and Machine Learning SI151

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Today:

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

Readings:

- The Element of Statistical Learning, Chapters 4.3, 4.4, 18.1, 18.2 and 18.3

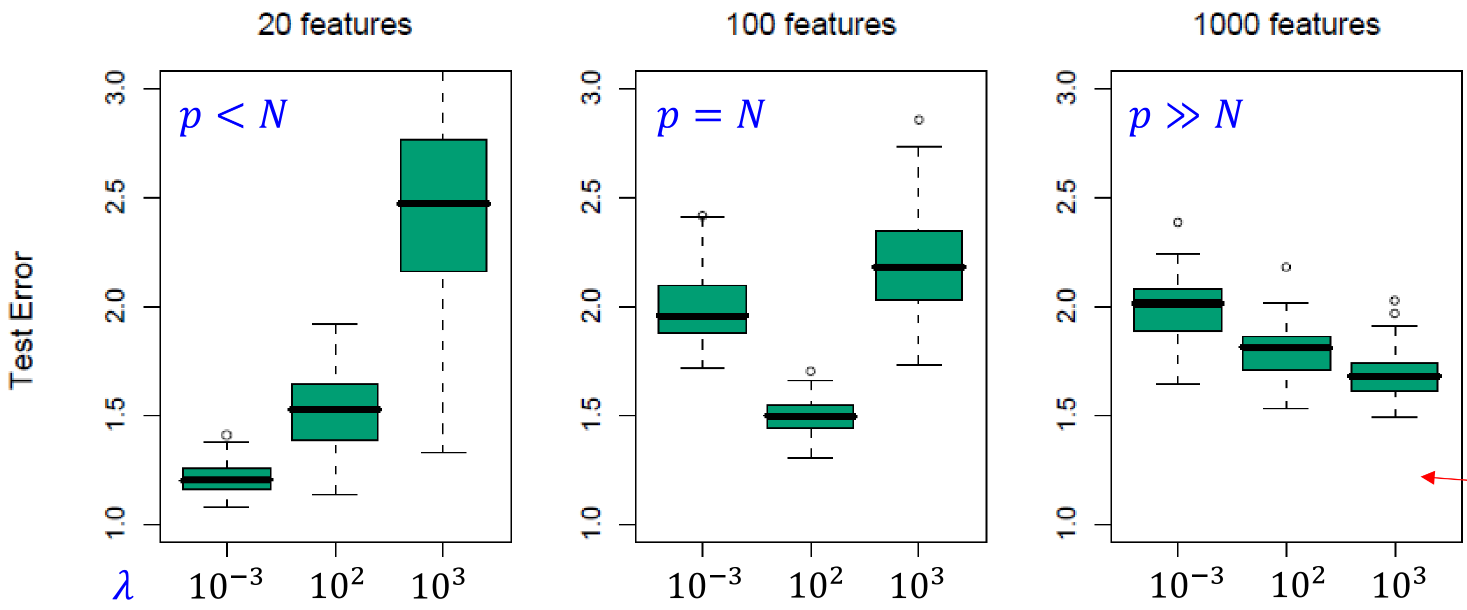
Linear Methods for Classification II

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

Regularized Discriminant Analysis

High dimensional problems ($p \gg N$)

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



Example

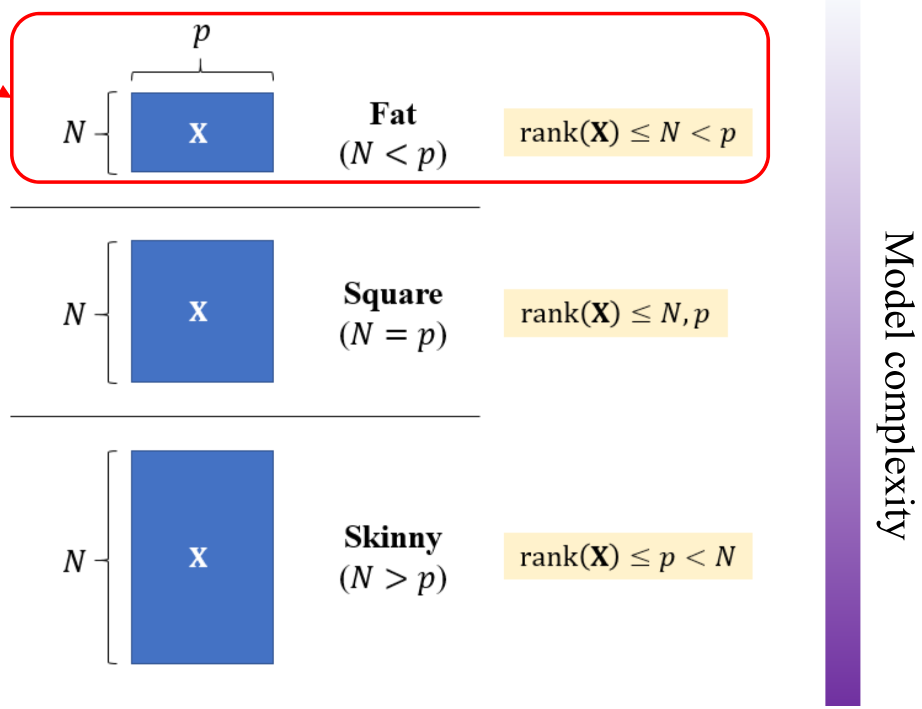
- 100 samples are generated by a linear model
- Ridge regression
- Relative error (divide by Bayes error)

No enough information to estimate the high-dimensional covariance matrix

Regularized Discriminant Analysis

High dimensional problems ($p \gg N$)

- Cannot fit LDA to the data
  - inversion of a $p \times p$ covariance matrix Σ
  - Σ is singular, due to $\mathrm{rank}(\Sigma) < N \ll p$
- 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 Discriminant Analysis

Regularized LDA (RLDA)

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

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

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

Diagonal LDA

- Independent assumption on feature dependencies

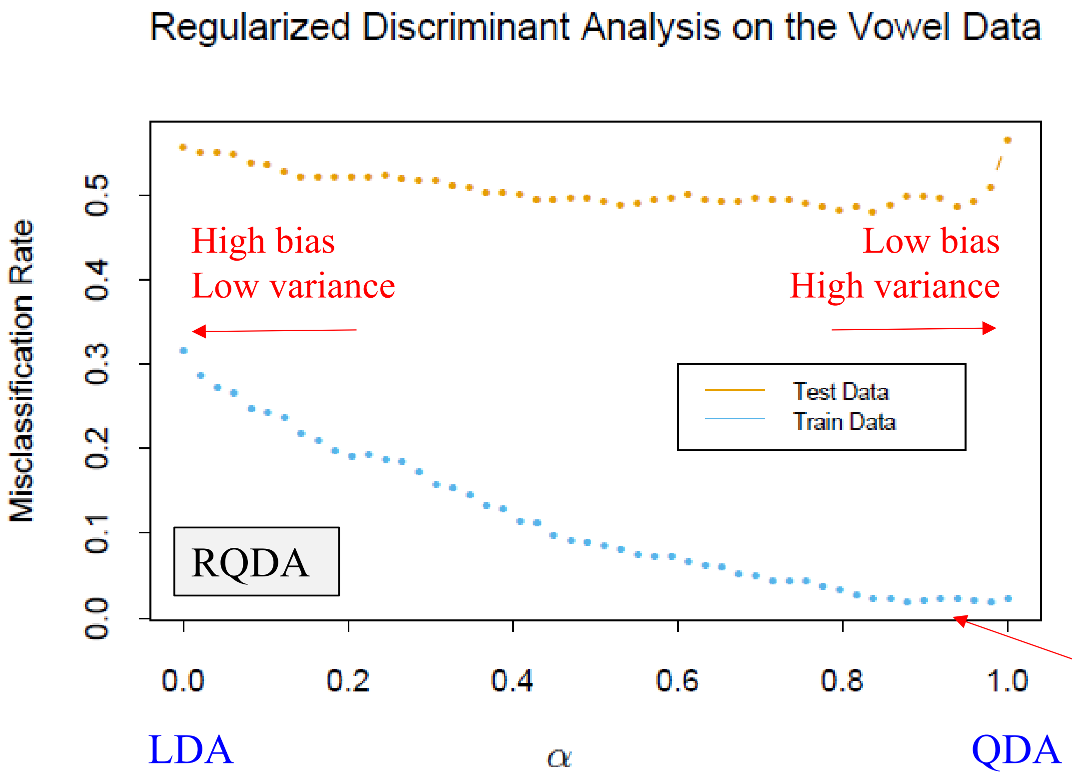
$$\hat{\Sigma} = \mathrm{diag}\big(\hat{\Sigma}\big)$$

Regularized Discriminant Analysis

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

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

Regularized Discriminant Analysis



RQDA:

$\hat{\Sigma}_k(\alpha) = \alpha\hat{\Sigma}_k + (1-\alpha)\hat{\Sigma}$

- $\alpha = 0$, LDA
- $\alpha = 1$, QDA

The optimal model

A compromise between QDA and LDA

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 $\boxed{\alpha = 0.9,}$ close to quadratic discriminant analysis.*

Regularized Discriminant Analysis

$\mathrm{diag}(\hat{\Sigma})$		$\hat{\Sigma}(\gamma)$		$\hat{\Sigma}$		$\hat{\Sigma}_k(\alpha)$		$\hat{\Sigma}_k$
Diagonal LDA	$\rightarrow$	RLDA	$\rightarrow$	LDA	$\rightarrow$	RQDA	$\rightarrow$	QDA

High bias
Low variance

Low bias
High variance

Fisher's Formulation of Discriminant Analysis

LDA: Approach 1

1. Estimating $\widehat{\boldsymbol{\Sigma}}$, $\hat{\mu}_k$ and $\hat{\pi}_k$
2. Discriminant function
   $$\delta_k(x) = x^T\widehat{\boldsymbol{\Sigma}}^{-1}\hat{\mu}_k - \frac{1}{2}\hat{\mu}_k^T\widehat{\boldsymbol{\Sigma}}^{-1}\hat{\mu}_k + \log\hat{\pi}_k$$
3. Classify to class k that maximizes the discriminant function
   $$\hat{G}(x) = \underset{k\in\mathcal{G}}{\operatorname{argmax}}\,\delta_k(x)$$

LDA: Approach 2

1. Estimating $\widehat{\boldsymbol{\Sigma}}$, $\hat{\mu}_k$ and $\hat{\pi}_k$
2. Eigen-decomposition:
   $$\widehat{\boldsymbol{\Sigma}} = \mathbf{UDU}^T$$
3. Data sphering ($\widehat{\Sigma}^* = \mathbf{I}$)
   - $x^* = \mathbf{D}^{-\frac{1}{2}}\mathbf{U}^T x = \widehat{\boldsymbol{\Sigma}}^{-\frac{1}{2}}x$
   - $\hat{\mu}_k^* = \mathbf{D}^{-\frac{1}{2}}\mathbf{U}^T\hat{\mu}_k = \widehat{\boldsymbol{\Sigma}}^{-\frac{1}{2}}\hat{\mu}_k$
4. Classify to its closest class centroid in the transformed space
   $$G(x) = \underset{k\in\mathcal{G}}{\operatorname{argmin}}\frac{1}{2}\|x^* - \hat{\mu}_k^*\|^2 - \ln\hat{\pi}_k$$

Q: why data sphering makes $\widehat{\boldsymbol{\Sigma}}^* = \mathbf{I}$?

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

Fisher's Formulation of Discriminant Analysis

LDA: Approach 1

1. Estimating $\widehat{\mathbf{\Sigma}}$, $\hat{\mu}_k$ and $\hat{\pi}_k$
2. Discriminant function
   $$\delta_k(x) = x^T \widehat{\mathbf{\Sigma}}^{-1} \hat{\mu}_k - \frac{1}{2} \hat{\mu}_k^T \widehat{\mathbf{\Sigma}}^{-1} \hat{\mu}_k + \log \hat{\pi}_k$$
3. Classify to class k that maximizes the discriminant function
   $$\boxed{\hat{G}(x) = \operatorname*{argmax}_{k \in \mathcal{G}} \delta_k(x)}$$

LDA: Approach 2

1. Estimating $\widehat{\mathbf{\Sigma}}$, $\hat{\mu}_k$ and $\hat{\pi}_k$
2. Eigen-decomposition:
   $$\widehat{\mathbf{\Sigma}} = \mathbf{U}\mathbf{D}\mathbf{U}^T$$
3. Data sphering ($\hat{\Sigma}^* = \mathbf{I}$)
   - $x^* = \mathbf{D}^{-\frac{1}{2}} \mathbf{U}^T x = \widehat{\mathbf{\Sigma}}^{-\frac{1}{2}} x$
   - $\hat{\mu}_k^* = \mathbf{D}^{-\frac{1}{2}} \mathbf{U}^T \hat{\mu}_k = \widehat{\mathbf{\Sigma}}^{-\frac{1}{2}} \hat{\mu}_k$
4. Classify to its closest class centroid in the transformed space
   $$\boxed{\hat{G}(x) = \operatorname*{argmin}_{k \in \mathcal{G}} \frac{1}{2} \|x^* - \hat{\mu}_k^*\|^2 - \ln \hat{\pi}_k}$$

Fisher's Formulation of Discriminant Analysis

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

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

$$\Pr(G = k|X = x) = \frac{\underbrace{\boxed{\Pr(X = x|G = k)}}_{\mathcal{N}(\hat{\mu}_k, \widehat{\boldsymbol{\Sigma}})}\underbrace{\boxed{\Pr(G = k)}}_{\hat{\pi}_k}}{\Pr(X = x)}$$

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

Constant

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

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

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

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

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

Fisher's Formulation of Discriminant Analysis

LDA: Approach 1

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

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

3. Classify to class k that maximizes the discriminant function

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

Complexity
$\mathcal{O}(p^3)$

LDA: Approach 2

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

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

3. Data sphering ($\hat{\Sigma}^* = \mathbf{I}$)
   - $x^* = \mathbf{D}^{-\frac{1}{2}} \mathbf{U}^T x = \widehat{\mathbf{\Sigma}}^{-\frac{1}{2}} x$
   - $\hat{\mu}_k^* = \mathbf{D}^{-\frac{1}{2}} \mathbf{U}^T \hat{\mu}_k = \widehat{\mathbf{\Sigma}}^{-\frac{1}{2}} \hat{\mu}_k$
4. Classify to its closest class centroid in the transformed space

$$\hat{G}(x) = \underset{k \in \mathcal{G}}{\operatorname{argmin}} \frac{1}{2} \|x^* - \hat{\mu}_k^*\|^2 - \ln \hat{\pi}_k$$

- Two approaches have almost the same time and storage complexity
- Approach 2 shows the potential of LDA for dimension reduction

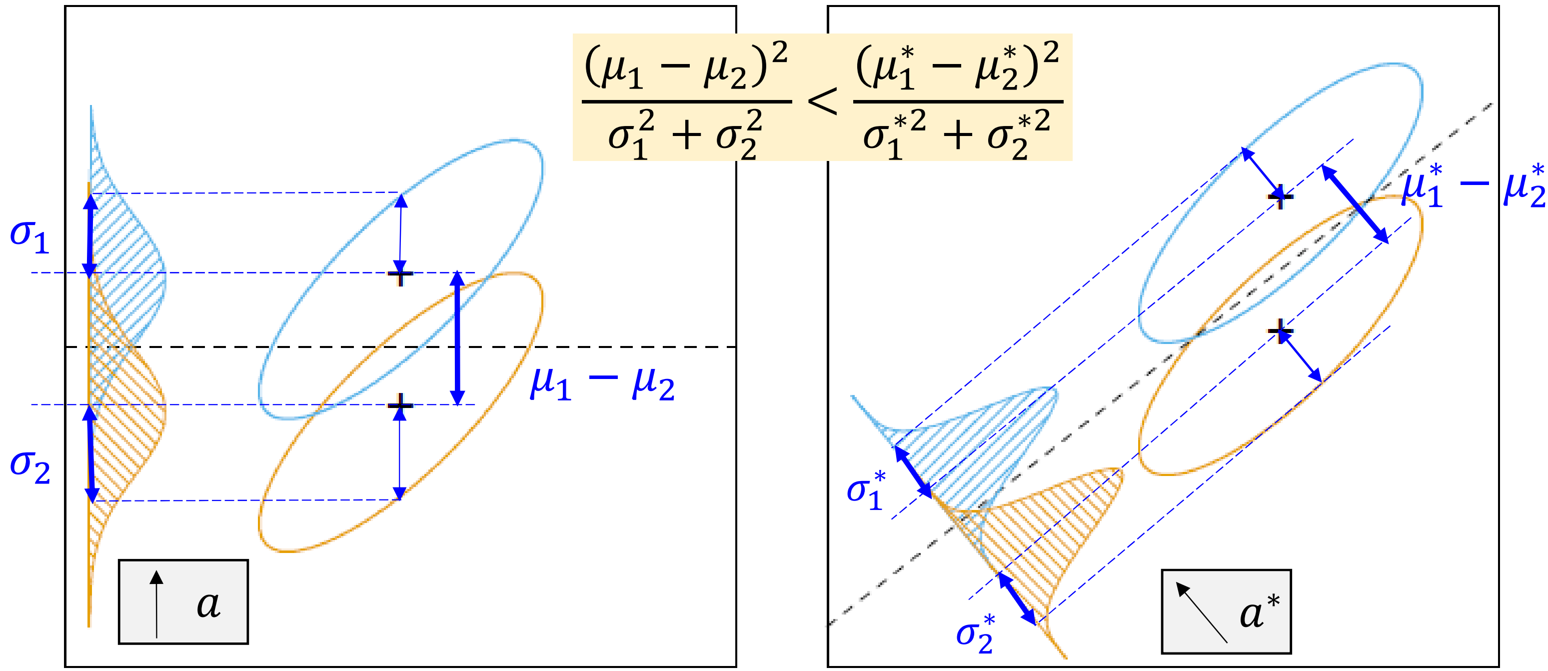
Fisher's Formulation of Discriminant Analysis

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

Between class variance

Our goal: $\max_a \dfrac{\boxed{(\mu_1^* - \mu_2^*)^2}}{\boxed{\sigma_1^{*2} + \sigma_2^{*2}}}$

Within class variance



Fisher's Formulation of Discriminant Analysis

- Maximize the Rayleigh quotient:

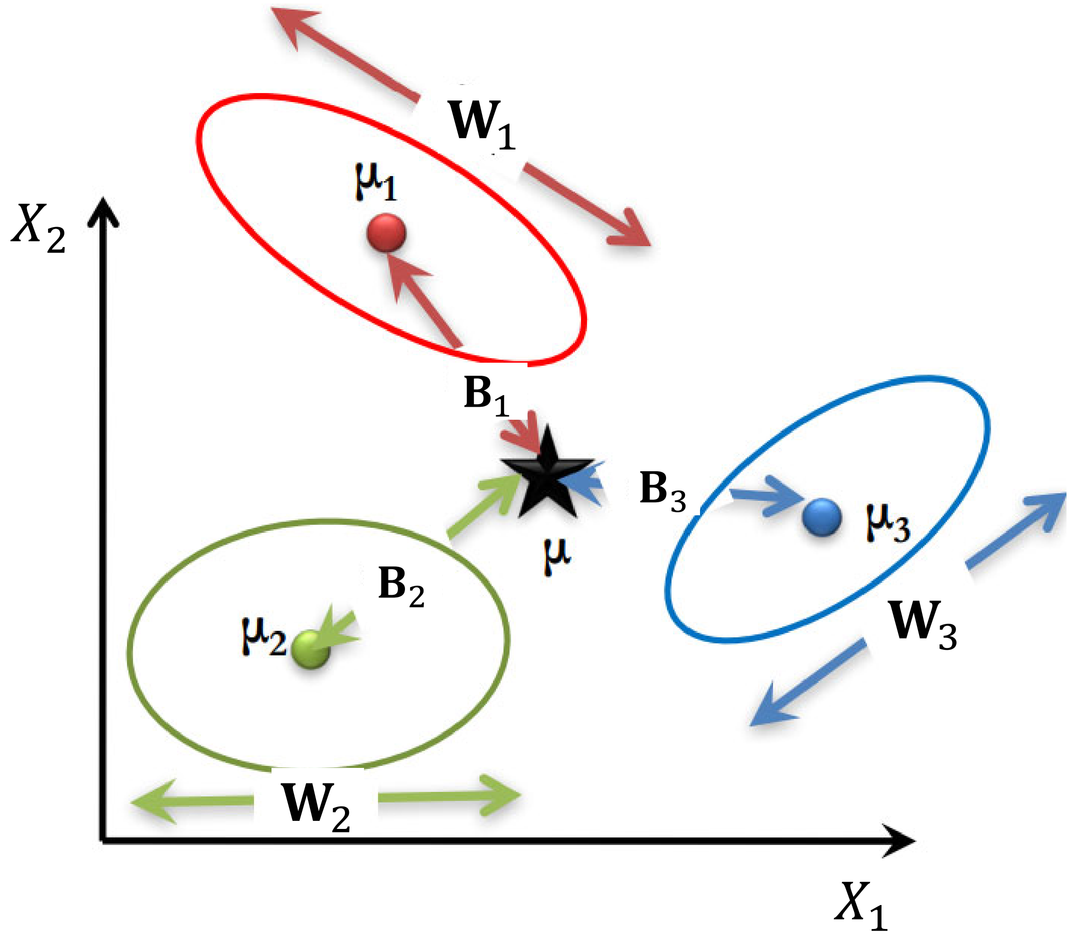
$$\max_a \frac{a^T \mathbf{B} a}{a^T \mathbf{W} a}$$

  - Between class variance

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

  - Within class variance

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



Fisher's Formulation of Discriminant Analysis

- 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,

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

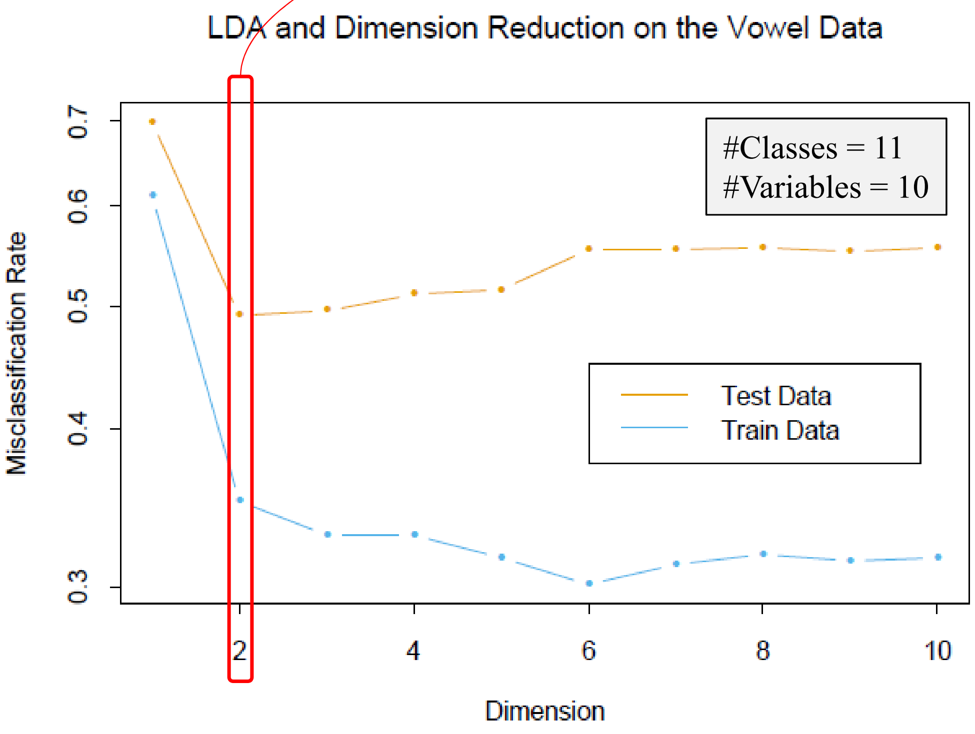
  - a is discriminant coordinates (canonical variates)
  - Generalized eigenvalue problem

$$\mathbf{B} a = \lambda \mathbf{W} a$$

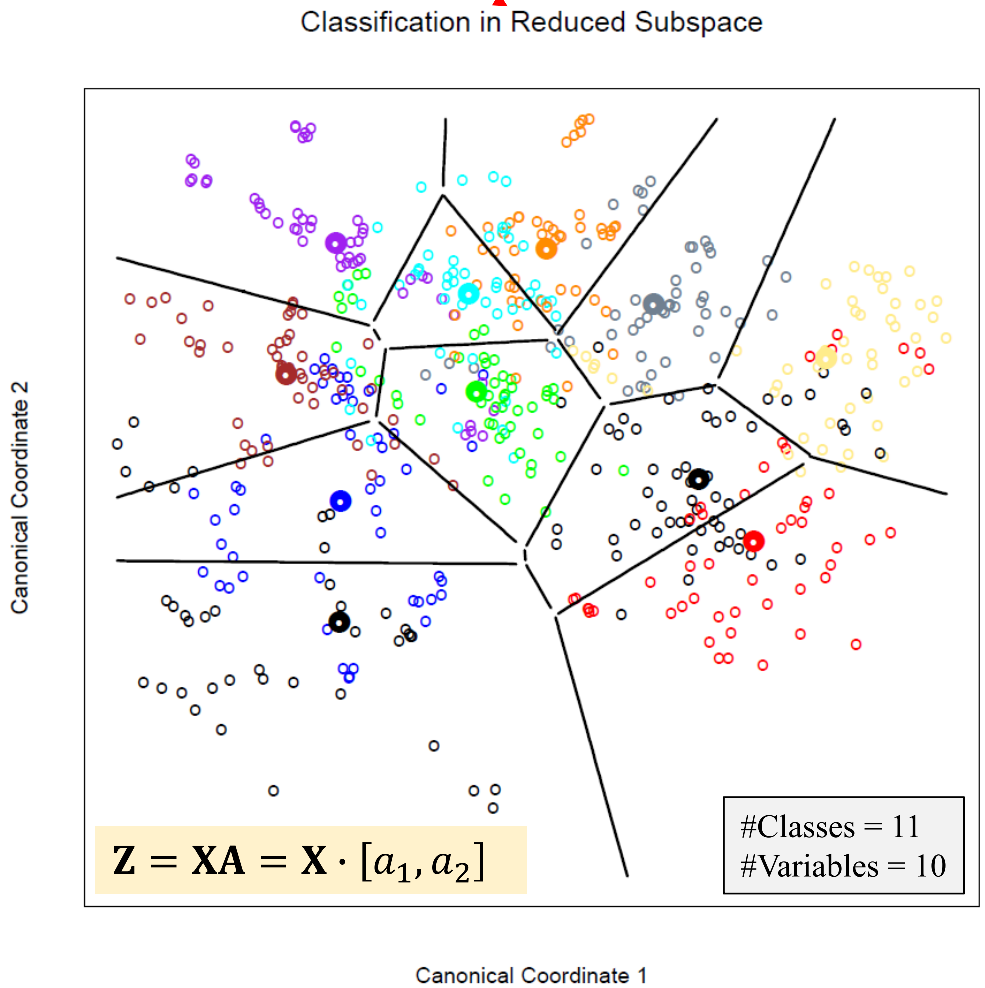
which can be efficiently solved

Ex. 4.1.
Hint: Lagrangian multipliers

Fisher's Formulation of Discriminant Analysis



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



$$\mathbf{Z} = \mathbf{X}\mathbf{A} = \mathbf{X} \cdot [a_1, a_2]$$

Fisher’s Formulation of Discriminant Analysis

We will discuss an example in our **live lecture** according to:

http://www.sci.utah.edu/~shireen/pdfs/tutorials/Elhabian_LDA09.pdf

Linear Methods for Classification II

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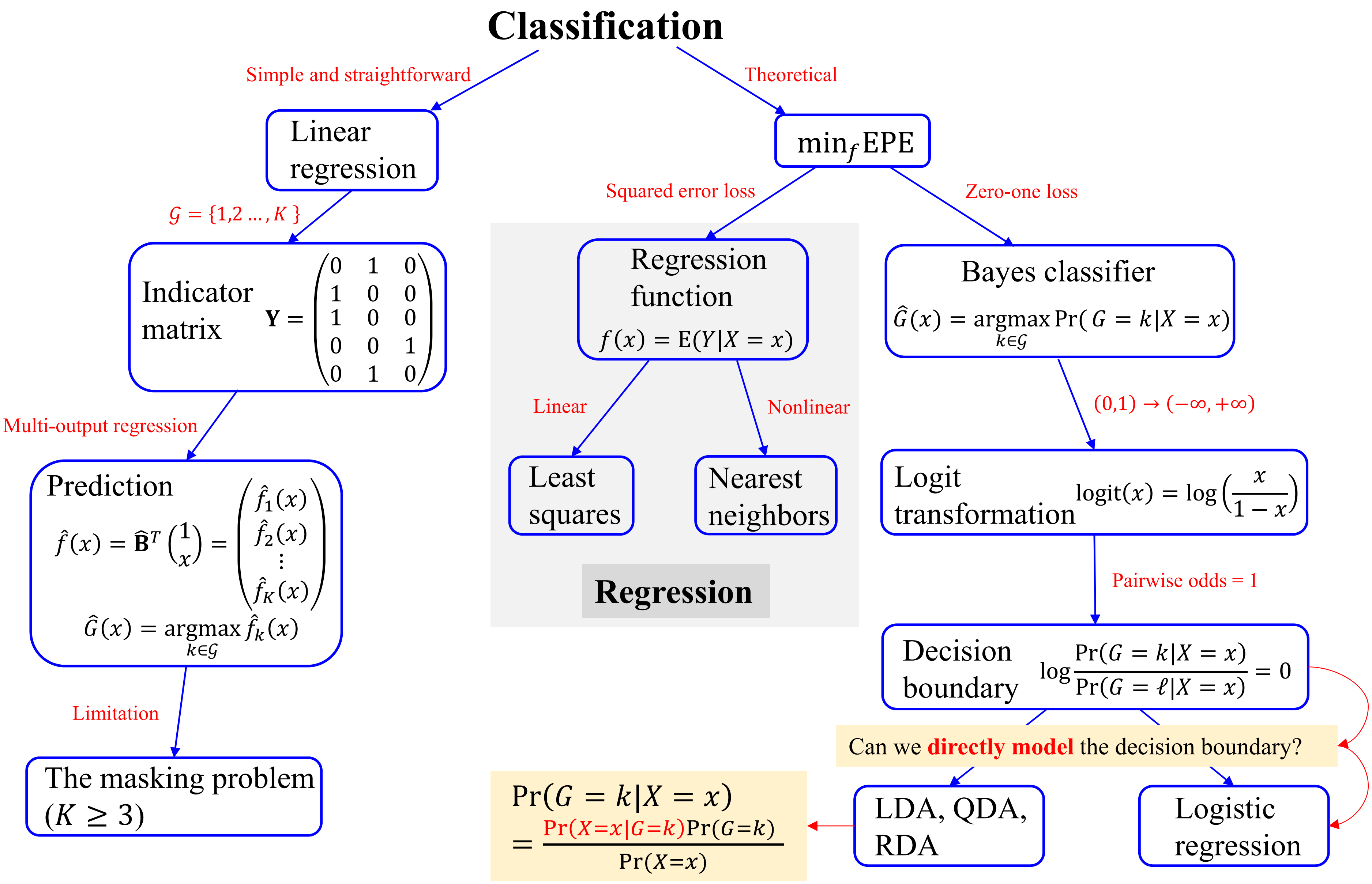
  - Fisher’s Formulation of Discriminant Analysis
- Logistic Regression
- Summary



Classification
Simple and straightforward
Theoretical
Linear regression
$\min_f \mathrm{EPE}$
$\mathcal{G} = \{1,2 \ldots, K\}$
Squared error loss
Zero-one loss
Indicator matrix
$\mathbf{Y} = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}$
Regression function
$f(x) = \mathrm{E}(Y|X = x)$
Bayes classifier
$\hat{G}(x) = \operatorname{argmax}_{k \in \mathcal{G}} \Pr(G = k|X = x)$
Multi-output regression
Linear
Nonlinear
$(0,1) \to (-\infty, +\infty)$
Prediction
$\hat{f}(x) = \hat{\mathbf{B}}^T \begin{pmatrix} 1 \\ x \end{pmatrix} = \begin{pmatrix} \hat{f}_1(x) \\ \hat{f}_2(x) \\ \vdots \\ \hat{f}_K(x) \end{pmatrix}$
$\hat{G}(x) = \operatorname{argmax}_{k \in \mathcal{G}} \hat{f}_k(x)$
Least squares
Nearest neighbors
Logit transformation
$\mathrm{logit}(x) = \log\left(\frac{x}{1-x}\right)$
Regression
Pairwise odds = 1
Limitation
Decision boundary
$\log \frac{\Pr(G = k|X = x)}{\Pr(G = \ell|X = x)} = 0$
Can we **directly model** the decision boundary?
The masking problem ($K \geq 3$)
$\Pr(G = k|X = x) = \frac{\Pr(X=x|G=k)\Pr(G=k)}{\Pr(X=x)}$
LDA, QDA, RDA
Logistic regression

Linear Logistic Regression

- 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

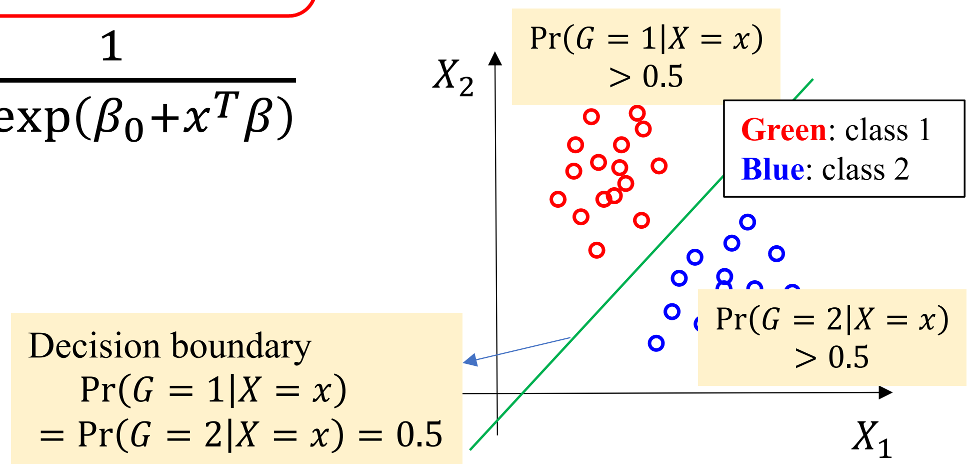
$$\Pr(G = 1|X = x) = \boxed{\frac{\exp(\beta_0+x^T\beta)}{1+\exp(\beta_0+x^T\beta)}},$$

logistic$(x^T\beta)$
$(-\infty, +\infty) \to (0,1)$

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

- Decision boundary

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



Linear Logistic Regression

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

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

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

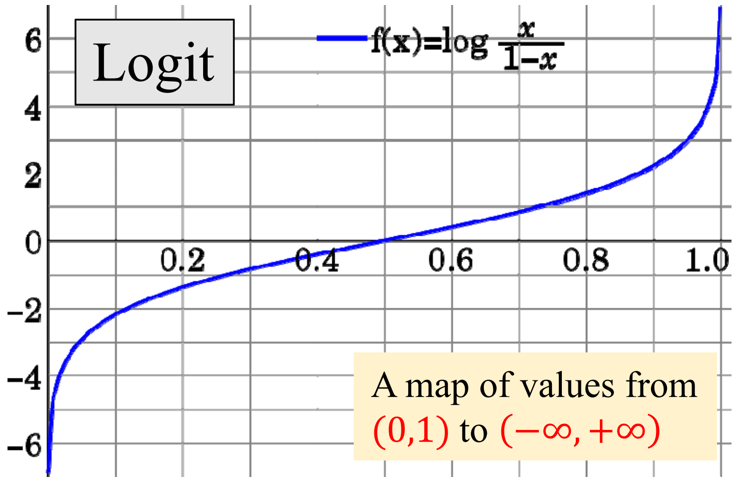
$$\vdots$$

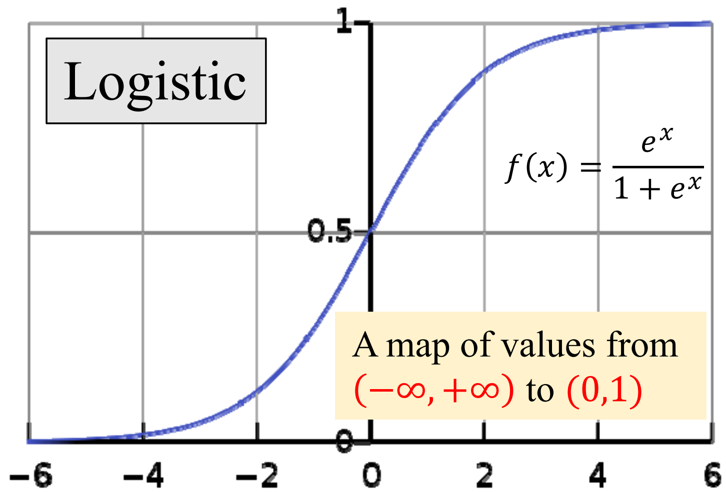
$$\log \frac{\Pr(G=K-1|X=x)}{\Pr(G=K|X=x)} = \beta_{(K-1)0} + x^T\beta_{K-1}$$

- $K-1$ log-odds or logit function

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

- The inverse of logit is logistic function





Linear Logistic Regression

- 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

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

- The inverse of logit is logistic function

?

- A simple calculation yields

$$\Pr(G=k|X=x) = \frac{\exp(\beta_{k0} + x^T\beta_k)}{1 + \sum_{\ell=1}^{K-1} \exp(\beta_{\ell 0} + x^T\beta_\ell)},$$

$$k = 1, \dots, K-1$$

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

- Parameter set

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

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

Linear Logistic Regression

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

$$\vdots$$

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

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

$$\vdots$$

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

summation

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

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

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

$$\Pr(G=k|X=x)=\frac{\exp(\beta_{k0}+x^T\beta_k)}{1+\sum_{\ell=1}^{K-1}\exp(\beta_{\ell 0}+x^T\beta_\ell)},k=1,\dots,K-1$$

Linear Logistic Regression

- Estimating parameter set $\theta = \{\beta_{10}, \beta_1, \ldots, \beta_{(K-1)0}, \beta_{K-1}\}$
  - 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	$p(x;\theta)$	$1 - p(x;\theta)$

Linear Logistic Regression

- Two classes

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

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

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

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

$$x_i \leftarrow \begin{pmatrix} 1 \\ x_i \end{pmatrix} \qquad \beta \leftarrow \begin{pmatrix} \beta_0 \\ \beta \end{pmatrix}$$

Linear Logistic Regression

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 *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)

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

- 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 $p(x_i)(1 - p(x_i))$

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

- The Newton-Raphson step:

$$\beta^{\text{new}} = \beta^{\text{old}} - \left(\frac{\partial^2 \ell(\beta)}{\partial \beta \partial \beta^T} \right)^{-1} \frac{\partial \ell(\beta)}{\partial \beta}$$
$$= \beta^{\text{old}} + (\mathbf{X}^T\mathbf{W}\mathbf{X})^{-1}\mathbf{X}^T(\mathbf{y} - \mathbf{p})$$
$$= (\mathbf{X}^T\mathbf{W}\mathbf{X})^{-1}\mathbf{X}^T\mathbf{W}\left(\mathbf{X}\beta^{\text{old}} + \mathbf{W}^{-1}(\mathbf{y} - \mathbf{p}) \right)$$
$$= (\mathbf{X}^T\mathbf{W}\mathbf{X})^{-1}\mathbf{X}^T\mathbf{W}\mathbf{z}$$

- Given the response

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

- it is represented as a weighted least squares problem:

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

Linear Logistic Regression

- Iteratively reweighted least squares (IRLS) algorithm

1. Initialize β
2. *Repeat*
3. Form linearized responses

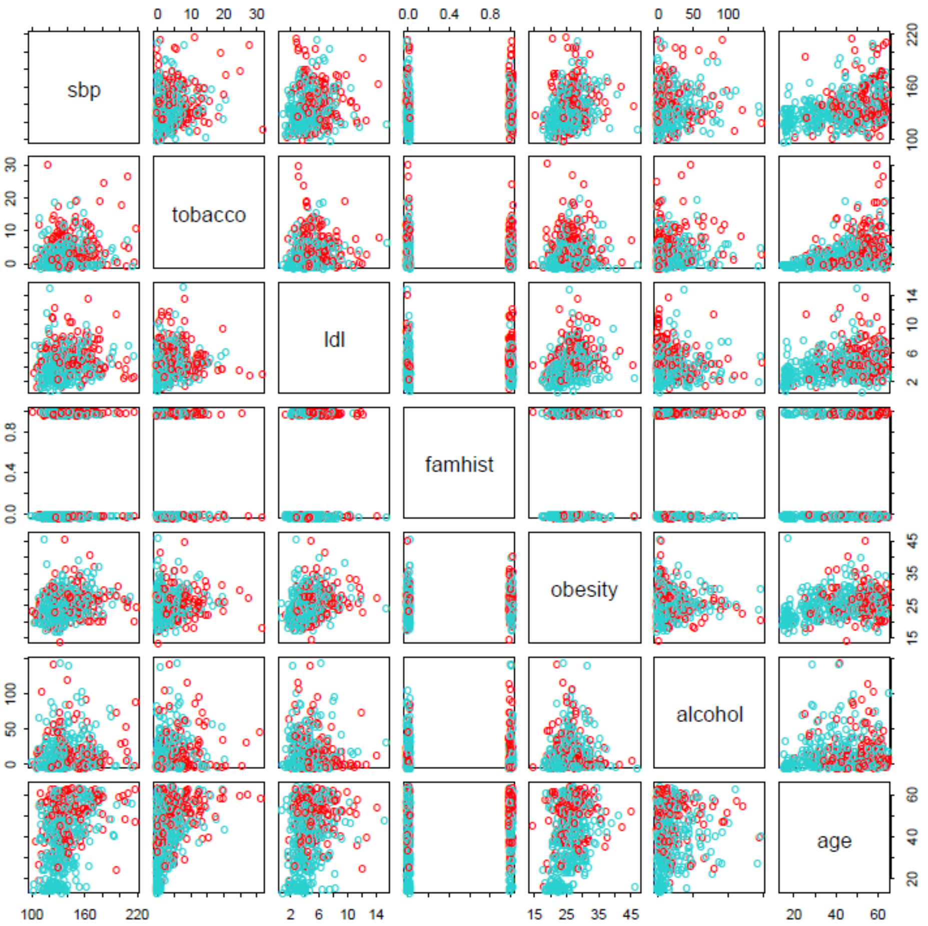
$$z_i = x_i^T \beta + \frac{y_i - p_i}{p_i(1 - p_i)}$$

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

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, $\forall i$
6. *Until convergence*

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

Linear Logistic Regression



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

Linear Logistic Regression

- L_1 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?

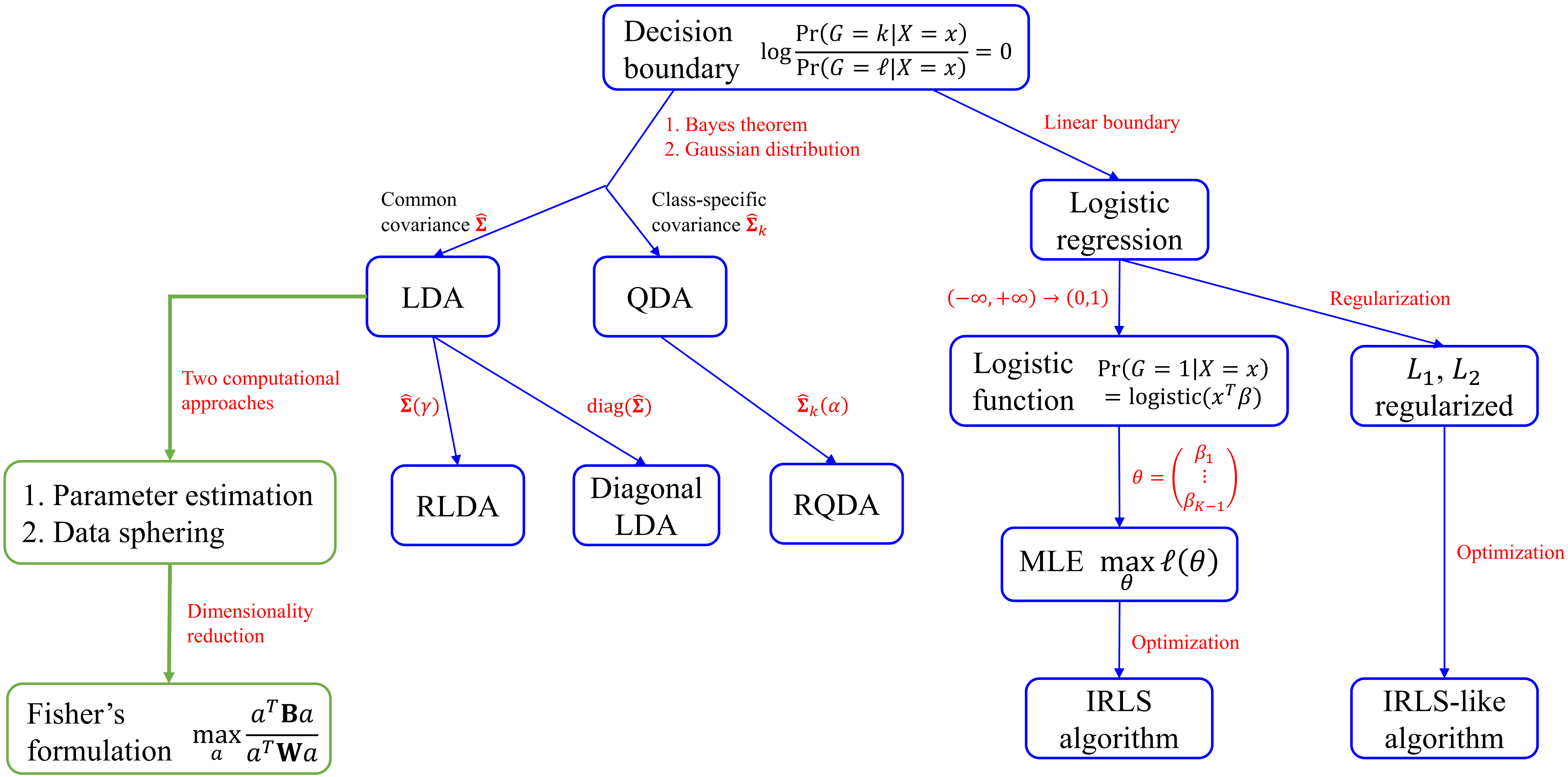
Connection between LDA and Logistic Regression

We will discuss the following example in our **live lecture**:

https://online.stat.psu.edu/stat508/lesson/9/9.2/9.2.9

Linear Methods for Classification II

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



Decision boundary $\log \frac{\Pr(G=k|X=x)}{\Pr(G=\ell|X=x)} = 0$
1. Bayes theorem
2. Gaussian distribution
Linear boundary
Common covariance $\hat{\mathbf{\Sigma}}$
Class-specific covariance $\hat{\mathbf{\Sigma}}_k$
Logistic regression
LDA
QDA
$(-\infty, +\infty) \to (0,1)$
Regularization
Two computational approaches
$\hat{\mathbf{\Sigma}}(\gamma)$
diag($\hat{\mathbf{\Sigma}}$)
$\hat{\mathbf{\Sigma}}_k(\alpha)$
Logistic function $\Pr(G=1|X=x) = \mathrm{logistic}(x^T\beta)$
L_1, L_2 regularized
1. Parameter estimation
2. Data sphering
RLDA
Diagonal LDA
RQDA
$\theta = \begin{pmatrix} \beta_1 \\ \vdots \\ \beta_{K-1} \end{pmatrix}$
MLE $\max_\theta \ell(\theta)$
Optimization
Dimensionality reduction
Optimization
Fisher's formulation $\max_a \frac{a^T\mathbf{B}a}{a^T\mathbf{W}a}$
IRLS algorithm
IRLS-like algorithm