Generative Classifiers

LDQ, QDA, Naive Bayes DS 6030 | Fall 2022

gen-classifiers.pdf

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1 Classification and Pattern Recognition

- The outcome variable is categorical and denoted $G \in \mathcal{G}$
 - Default Credit Card Example: $\mathcal{G} = \{\text{"Yes", "No"}\}\$
 - Medical Diagnosis Example: $\mathcal{G} = \{\text{"stroke", "heart attack", "drug overdose", "vertigo"}\}$
- The training data is $D = \{(X_1, G_1), (X_2, G_2), \dots, (X_n, G_n)\}$
- The optimal decision/classification is often based on the posterior probability $Pr(G = g \mid \mathbf{X} = \mathbf{x})$

1.1 Binary Classification

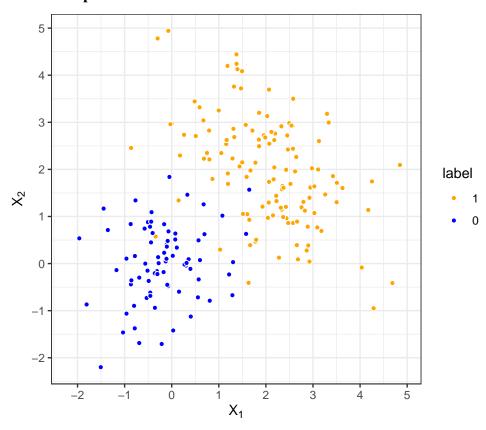
- Classification is simplified when there are only 2 classes.
 - Many multi-class problems can be addressed by solving a set of binary classification problems (e.g., one-vs-rest).
- It is often convenient to transform the outcome variable to a binary $\{0,1\}$ variable:

$$Y_i = \begin{cases} 1 & G_i = \mathcal{G}_1 \\ 0 & G_i = \mathcal{G}_2 \end{cases}$$
 (outcome of interest)

• Or, like with SVM, as a $\{-1, +1\}$ variable:

$$Y_i = \begin{cases} +1 & G_i = \mathcal{G}_1 \\ -1 & G_i = \mathcal{G}_2 \end{cases}$$
 (outcome of interest)

1.2 Two-Class Example



1.3 Discriminative Models

- The models we have covered in this course so far (Linear Regression, Logistic Regression, SVM, and KNN) can be considered *discriminative* models.
- Their goal is to directly estimate $Pr(Y = 1 \mid X = x)$ conditional on X = x.

$$p(x) = \Pr(Y = 1 \mid X = x)$$

a. Linear Regression (for binary outcomes)

$$\hat{p}(x) = \hat{\beta}^{\mathsf{T}} x$$

b. Logistic Regression

$$\log\left(\frac{\hat{p}(x)}{1-\hat{p}(x)}\right) = \hat{\beta}^{\mathsf{T}} x$$

and thus,

$$\hat{p}(x) = \frac{e^{\hat{\beta}^\mathsf{T} x}}{1 + e^{\hat{\beta}^\mathsf{T} x}}$$
$$= \left(1 + e^{-\hat{\beta}^\mathsf{T} x}\right)^{-1}$$

c. kNN (for binary outcomes)

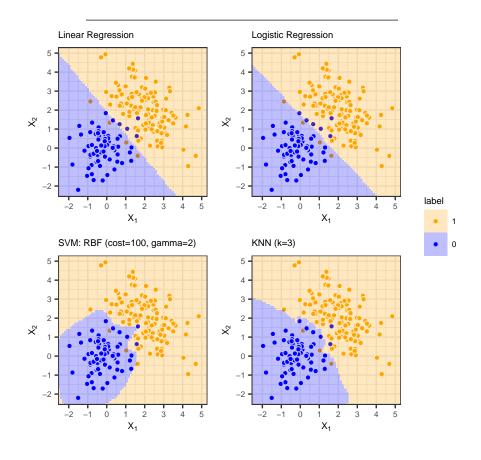
$$\hat{p}(x;k) = \frac{1}{k} \sum_{i:x_i \in N_k(x)} y_i$$
$$= \text{Avg}(y_i \mid x_i \in N_k(x))$$

• $N_k(x)$ are the set of k nearest neighbors

d. Support Vector Machines (SVM)

$$\hat{g}(x) = \hat{\beta}_0 + \sum_{i=1}^n \hat{\alpha}_i y_i K(x, x_i)$$

- Decide $\hat{Y} = 1$ if $\hat{g}(x) > 0$
- Or calibrated probability: $\log \frac{\hat{p}(x)}{1-\hat{p}(x)} = \hat{\alpha}_0 + \hat{\alpha}_1 \hat{g}(x)$
 - I.e., using logistic regression with $\hat{g}(x)$ as the predictor.



2 Generative Classification Models

Consider how the data $D = \{(X_1, G_1), (X_2, G_2), \dots, (X_n, G_n)\}$ could be generated.

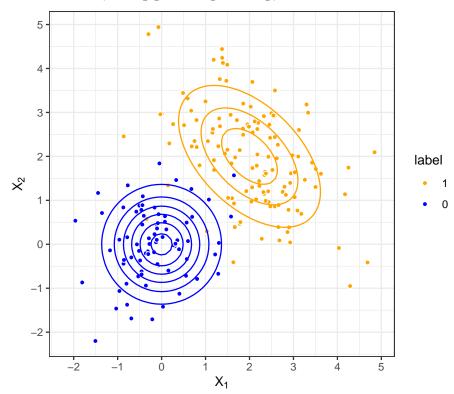
- 1. First, the class label is selected according to the *prior probabilities* $\pi = [\pi_1, \dots, \pi_K]$.
 - That is, $Pr(G_i = k) = \pi_k$
- 2. Given the class is k, the X value is generated $X \mid G = k \sim f_k$
 - Let $f_k(\mathbf{x})$ be the (pdf/pmf/mixed) of the predictors from class k.
- 3. Repeat n times

Example

- Two classes, $k \in \{0, 1\}$
 - $-\pi_1 = 0.6, \pi_0 = 0.4$
 - I expect 60% of the observations to be from class 1.

• If
$$G_i = 1$$
, then $X \sim N \left(\mu_1 = \begin{bmatrix} 2 \\ 2 \end{bmatrix}, \Sigma_1 = \begin{bmatrix} 1 & -0.5 \\ -0.5 & 1 \end{bmatrix} \right)$

• If
$$G_i=0$$
, then $X\sim N\left(\mu_0=\begin{bmatrix}0\\0\end{bmatrix}, \Sigma_0=\begin{bmatrix}0.5&0\\0&0.5\end{bmatrix}\right)$



- The models we have discussed in this course so far are considered *discriminative* and focused on estimating the **conditional** probability $Pr(Y = k \mid X = x)$
- But there is another class of models termed *generative* which try to directly estimate the **joint** probability $Pr(Y = k, X = x) = Pr(X = x \mid Y = k) Pr(Y = k)$

2.1.1 The Bayes Breakdown (Binary Classification)

Bayes Theorem

$$p(x) = \Pr(Y = 1 \mid X = x) = \frac{\Pr(X = x \mid Y = 1) \Pr(Y = 1)}{\Pr(X = x)}$$
$$= \frac{f_1(x)\pi}{f_1(x)\pi + f_0(x)(1 - \pi)}$$

- $f_k(x)$ is the class conditional density
- $0 \le \pi_k \le 1$ are the prior class probabilities
- $\pi_0 + \pi_1 = 1$
- X is distributed as a finite mixture model

-
$$f(x) = \sum_{j} f_j(x) \pi_j$$

Recall our notation for the log-odds:

•
$$\gamma(x) = \log \frac{p(x)}{1 - p(x)}$$

The log-odds reduces to a combination of prior odds and density ratios

$$\begin{split} \gamma(x) &= \log \left(\frac{p(x)}{1 - p(x)} \right) \\ &= \log \left(\frac{f_1(x)\pi}{f_0(x)(1 - \pi)} \right) \\ &= \underbrace{\log \left(\frac{\pi}{1 - \pi} \right)}_{\text{log prior odds}} + \underbrace{\log \left(\frac{f_1(x)}{f_0(x)} \right)}_{\text{log density ratio}} \end{split}$$

2.1.2 Decision-Making (Hard Classification)

• We know that the optimal decision can be based on the density ratios

$$\begin{split} & \text{Choose } \hat{G}(x) = 1 \text{ if:} \\ & \hat{\gamma}(x) > \log \left(\frac{C_{\text{FP}}}{C_{\text{FN}}} \right) \\ & \log \left(\frac{1 - \hat{\pi}}{\hat{\pi}} \right) + \log \left(\frac{\widehat{f_1(x)}}{f_0(x)} \right) > \log \left(\frac{C_{\text{FP}}}{C_{\text{FN}}} \right) \\ & \log \left(\frac{\widehat{f_1(x)}}{f_0(x)} \right) > \log \left(\frac{1 - \hat{\pi}}{\hat{\pi}} \right) + \log \left(\frac{C_{\text{FP}}}{C_{\text{FN}}} \right) \end{split}$$

2.1.3 Estimation

- $\hat{\pi}_k = n_k/n$ is a natural estimate for the class priors if we think the testing data will have the same proportions as the training data
- The other term to estimate is the log density ratio: $\log \left(\frac{\widehat{f_1(x)}}{f_0(x)} \right)$
- Generative Models estimate this term by

$$\log\left(\frac{\widehat{f_1(x)}}{\widehat{f_0(x)}}\right) = \log\left(\frac{\widehat{f_1(x)}}{\widehat{f_0(x)}}\right)$$

- That is, generative models estimate the class conditional densities $\{f_k(\cdot)\}$
- The different generative models take different approaches to estimate these component densities

Generative Models

Generative Classification Models use *density estimation* to make predictions!

2.1.3.1 Linear/Quadratic Discriminant Analysis (LDA/QDA)

- Both LDA and QDA model the class conditional densities $f_k(x)$ with a Gaussian density
 - Thus, they model the observations as coming from a Gaussian mixture model
 - Each class has its own mean vector μ_k
 - The difference between LDA and QDA is what they use for their covariance matrix
- LDA

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

- $\Sigma_k = \Sigma$ $\forall k$ (uses the same variance-covariance for all classes)
- QDA

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

- \sum_{k} is different for each classes

2.1.3.2 Kernel Discriminant Analysis (KDA)

• Model the class conditional densities $f_k(x)$ with a multivariate kernel density estimate (KDE)

$$\hat{f}_k(x) = \frac{1}{n_k} \sum_{i:g_i = k} K(x - x_i; H)$$

where H is the $p \times p$ bandwidth matrix.

2.1.3.3 Mixture Discriminant Analysis (MDA)

• Model the class conditional densities $f_k(x)$ with a finite mixture model

$$\hat{f}_k(x) = \frac{1}{J} \sum_{j=1}^{J} \pi_j g_j(x; \theta_j)$$

where $\sum_{j=1}^{J} \pi_j = 1$ and $g_j(x)$ is a density function (e.g., Gaussian).

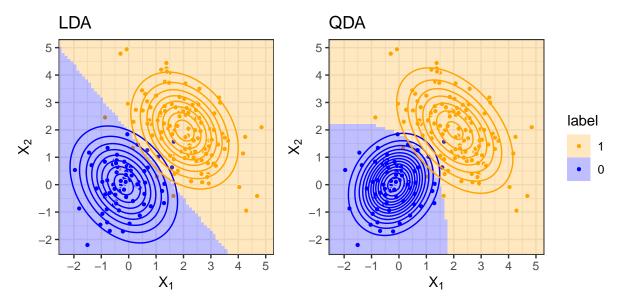
2.1.3.4 Naive Bayes

• Naive Bayes ignores potential associations between predictors and estimates the density of each predictor variable independently.

$$\hat{f}_k(x) = \prod_{j=1}^p \hat{f}_{jk}(x_j)$$

- This greatly simplifies the estimation
- You will often find $\hat{f}_{jk}(u) = \mathcal{N}(u; \hat{\mu}_{jk}, \hat{\sigma}_{jk})$
- But KDE is a great approach $\hat{f}_{jk}(u)=\frac{1}{n_k}\sum_{\{i:G_i=k\}}K_h(u-x_{ij})$ And mix continuous and discrete variables is very easily

3 Linear/Quadratic Discriminant Analysis (LDA/QDA)



- Linear Discriminant Analysis (LDA) finds linear boundaries between classes
- Quadratic Discriminant Analysis (QDA) finds quadratic boundaries between classes
- Setup: $K=|\mathcal{G}|$ classes in the training data, $D=\{(\mathbf{X}_i,G_i)\}_{i=1}^n$ where $\mathbf{X}_i\in\mathbf{R}^p,G_i\in\mathcal{G}$
- The posterior probability of class g, given X = x,

$$\Pr(G = g \mid \mathbf{X} = \mathbf{x}) = \frac{f(x \mid G = g) \Pr(G = g)}{f(x)}$$
$$= \frac{f_g(x) \pi_g}{\sum_{k=1}^K f_k(x) \pi_k}$$

- $f_k(x)$ is the class conditional density
- $0 \le \pi_k \le 1$ are the *prior class probabilities*; $\sum_{k=1}^K \pi_k = 1$

3.1 Estimation

- Both LDA and QDA model the class conditional densities $f_k(x)$ with Gaussians
 - Thus, they model the observations as coming from a K component Gaussian mixture model
 - Each class has its own mean vector μ_k
 - The difference between LDA and QDA is what they use for their covariance matrix

$$f_k(x) = \mathcal{N}(x; \mu_k, \Sigma_k)$$

- LDA: $\hat{\Sigma}_1 = \hat{\Sigma}_2 = \ldots = \hat{\Sigma}_K = \hat{\Sigma}$ Common covariance
- QDA: $\hat{\Sigma}_1 \neq \hat{\Sigma}_2 \neq ... \neq \hat{\Sigma}_K$ Different covariances
- LDA

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

- $\Sigma_k = \Sigma$ $\forall k$ (uses the same variance-covariance for all classes)

• QDA

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

- \sum_{k} is different for each classes

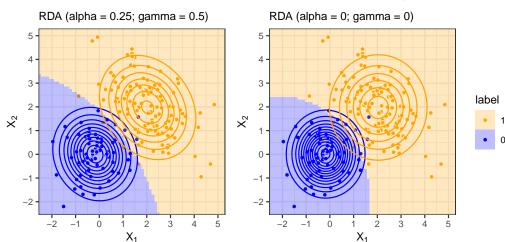
Your Turn #1: Model Complexity

The LDA model uses a common covariance matrix while QDA allows each class to have a different covariance (which permits quadratic boundaries). But this flexibility comes at a cost.

- 1. How many parameters have to be estimated in an LDA model with K classes and p dimensions?
- 2. How many parameters have to be estimated in an QDA model with K classes and p dimensions?

- There are a few methods to maintain some flexibility, yet protect the model from high variance
- One is to use a *regularlized covariance matrix* (see ESL 4.3.1). Called Regularlized Discriminant Analysis (RDA)

$$\hat{\Sigma}_k(\alpha, \gamma) = \alpha \hat{\Sigma}_k + (1 - \alpha) \{ \gamma \hat{\Sigma} + (1 - \gamma) \hat{\sigma}^2 I_p \}$$



• A special case of above using diagonal covariance matrices only $(\hat{\Sigma}_k(\alpha=0,\gamma=0))$. This covariance

matrix has all off-diagonal terms set to 0.

$$\hat{\Sigma}_k = diag(\hat{\sigma}_1^2, \hat{\sigma}_2^2, \dots, \hat{\sigma}_p^2)$$

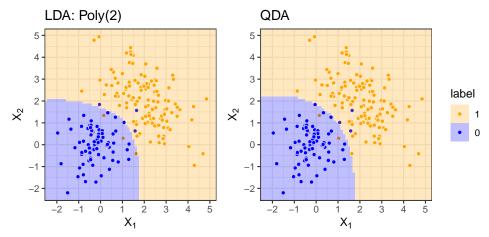
$$= \begin{bmatrix} \sigma_1^2 & 0 & \dots & 0 \\ 0 & \sigma_2^2 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & \sigma_p^2 \end{bmatrix}$$

- This treats predictors/features as uncorrelated/independent.
- It is a special case of Naive Bayes!
- A more restrictive (less complex) model specifies that variance in all dimensions are equal

$$\hat{\Sigma}_k = \hat{\sigma}^2 I_p$$

$$= \begin{bmatrix} \sigma^2 & 0 & \dots & 0 \\ 0 & \sigma^2 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & \sigma^2 \end{bmatrix}$$

- This treats predictors/features as uncorrelated/independent.
- It is a special case of Naive Bayes!
- Models all variances as equal.
- In some settings (large K, small p), edf could be reduced by fitting an LDA model in an *enlarged* feature space
 - E.g., for p=2 dimensions, use $X_1,X_2,X_1\cdot X_2,X_1^2,X_2^2$ instead of QDA in X_1,X_2 .
 - Think basis expansion like what we did with polynomial regression or B-splines
 - Or kernels with SVM



Mahalanobis Distance

Notice that a multivariate normal density is a function of the squared *Mahalanobis* distance from x to the mean.

$$f(\mathbf{x}) = (2\pi)^{-p/2} |\Sigma|^{-1/2} \exp\left\{-\frac{1}{2}(\mathbf{x} - \mu)^{\mathsf{T}} \Sigma^{-1}(\mathbf{x} - \mu)\right\}$$
$$= (2\pi)^{-p/2} |\Sigma|^{-1/2} \exp\left\{-\frac{1}{2} D_m^2(x)\right\}$$

where

$$D_m(x) = \sqrt{(\mathbf{x} - \mu)^{\mathsf{T}} \Sigma^{-1} (\mathbf{x} - \mu)}$$

is the Mahalanobis distance.

3.2 LDA/QDA in Action

- In **R**, LDA and QDA can be implemented with the lda() and qda() functions from the MASS package.
- See ISLR 4.7 for details
- Warning: the MASS package has a select() functions that conflicts with dplyr's select(). If you use tidyverse, I suggest you use MASS::lda() and MASS::qda() instead of loading the MASS package.

3.3 Connections: LDA, QDA, and Logistic Regression

ISL 4.5 and ESL 4.4.5 show more details about the parametric form LDA and QDA take.

Recall the notation for generative models:

$$\hat{\gamma}(x) = \log\left(\frac{\hat{p}(x)}{1 - \hat{p}(x)}\right)$$
$$= \log\left(\frac{\hat{\pi}}{1 - \hat{\pi}}\right) + \log\left(\frac{\hat{f}_1(x)}{\hat{f}_0(x)}\right)$$

Logistic Regression

$$\hat{\gamma}(x) = \hat{\beta}_0 + \sum_{j=1}^p \hat{\beta}_j x_j$$

LDA

$$\hat{\gamma}(x) = \hat{\alpha}_0 + \sum_{j=1}^p \hat{\alpha}_j x_j$$

$$\hat{a}_0 = \log \frac{\hat{\pi}}{1 - \hat{\pi}} - \frac{1}{2} (\hat{\mu}_1 - \hat{\mu}_0)^\mathsf{T} \hat{\Sigma}^{-1} (\hat{\mu}_1 - \hat{\mu}_0)$$

$$\hat{a}_j = \text{the } j \text{th element of } \hat{\Sigma}^{-1} (\hat{\mu}_1 - \hat{\mu}_0)$$

QDA

$$\begin{split} \hat{\gamma}(x) &= \hat{\alpha}_0 + \sum_{j=1}^p \hat{\alpha}_j x_j + \sum_{j=1}^p \sum_{k=1}^p \hat{a}_{jk} x_j x_k \\ \hat{a}_0 &= \log \frac{\hat{\pi}}{1 - \hat{\pi}} - \frac{1}{2} \log \frac{|\hat{\Sigma}_1|}{|\hat{\Sigma}_0|} - \frac{1}{2} \left(\hat{\mu}_1^\mathsf{T} \Sigma_1^{-1} - \hat{\mu}_0^\mathsf{T} \Sigma_0^{-1} \right) \\ \hat{a}_j &= \text{the } j \text{th element of } \hat{\Sigma}_1^{-1} \hat{\mu}_1 - \hat{\Sigma}_0^{-1} \hat{\mu}_0 \\ \hat{a}_{jk} &= \text{the } (j,k) \text{th element of } (\hat{\Sigma}_0^{-1} - \hat{\Sigma}_1^{-1})/2 \end{split}$$

3.3.1 Estimation

LDA and QDA estimates model parameters by maximizing the *joint* likelihood:

$$\begin{split} \hat{\alpha} &= \underset{\alpha}{\operatorname{arg\,max}} \ \operatorname{Pr}(X,Y) \\ &= \underset{\alpha}{\operatorname{arg\,max}} \ \operatorname{Pr}(X \mid Y) \operatorname{Pr}(Y) \\ &= \underset{\alpha}{\operatorname{arg\,max}} \ \operatorname{Pr}(Y \mid X) \operatorname{Pr}(X) \end{split}$$

Logistic Regression estimates model parameters by maximizing the conditional likelihood

$$\hat{\beta} = \mathop{\arg\max}_{\beta} \; \Pr(Y \mid X)$$

4 Kernel Discriminant Analysis (KDA)

• Model the class conditional densities $f_k(x)$ with a multivariate kernel density estimate (KDE)

$$f_k(x) = \frac{1}{n_k} \sum_{i:q_i = k} K(x - x_i; H)$$

where H is the $p \times p$ bandwidth matrix.

There are three primary approaches to multivariate (p dimensional) KDE:

- 1. Multivariate kernels
 - e.g., $K(u) = N(\mathbf{0}, H)$:

$$\hat{f}(x) = \frac{1}{(2\pi)^{d/2}|H|^{1/2}n} \sum_{i=1}^{n} \exp\left(-\frac{1}{2}(x-x_i)^{\mathsf{T}}H^{-1}(x-x_i)\right)$$

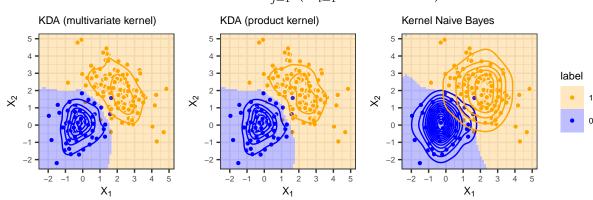
- 2. Product Kernels
 - $H = diag(h_1, h_2, \dots, h_p)$

$$\hat{f}(x) = \frac{1}{n} \sum_{i=1}^{n} \left(\prod_{j=1}^{p} K(x_j - x_{ij}; h_j) \right)$$

- 3. Independence
 - This is a special case of Naive Bayes (Kernel Naive Bayes)!

$$\hat{f}(x) = \prod_{j=1}^{p} \hat{f}_{j}(x)$$

$$= \prod_{j=1}^{p} \left(\frac{1}{n} \sum_{i=1}^{n} K(x_{j} - x_{ij}; h_{j}) \right)$$



4.1 KDA with R

• In **R**, the ks::kda() function (ks package) implements Kernel Discriminant Analysis.

5 Naive Bayes

Naive Bayes is a generative model that ignores potential associations between predictors and estimates the density of each predictor variable independently.

$$\hat{f}_k(x) = \prod_{j=1}^p \hat{f}_{kj}(x_j)$$

- This greatly simplifies the estimation
- The densities do *not* have to be Gaussian (e.g., KDE is a good option)
- Categorical densities (i.e., pmfs) can be thrown in the mix without a problem
- Because of the independence, this is easy to implement in parallel (and thus can be fast)
- The decision function becomes:

$$\hat{\gamma}(x) = \log\left(\frac{\hat{p}(x)}{1 - \hat{p}(x)}\right)$$

$$= \log\left(\frac{\hat{\pi}}{1 - \hat{\pi}}\right) + \log\left(\frac{\hat{f}_1(x)}{\hat{f}_0(x)}\right)$$

$$= \log\left(\frac{\hat{\pi}}{1 - \hat{\pi}}\right) + \log\left(\frac{\prod_{j=1}^p \hat{f}_{1j}(x_j)}{\prod_{j=1}^p \hat{f}_{0j}(x_j)}\right)$$

$$= \log\left(\frac{\hat{\pi}}{1 - \hat{\pi}}\right) + \log\left(\prod_{j=1}^p \frac{\hat{f}_{1j}(x_j)}{\hat{f}_{0j}(x_j)}\right)$$

$$= \log\left(\frac{\hat{\pi}}{1 - \hat{\pi}}\right) + \sum_{j=1}^p \log\left(\frac{\hat{f}_{1j}(x_j)}{\hat{f}_{0j}(x_j)}\right)$$

5.1 Gaussian Naive Bayes

• Recall in LDA/QDA, the class conditional densities were estimated as Gaussians:

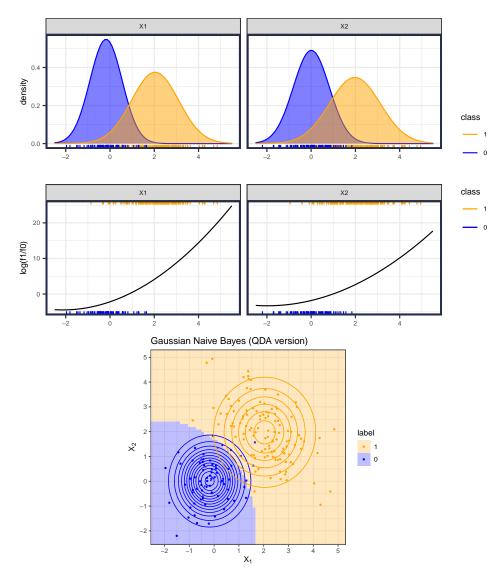
$$\hat{f}_k(\mathbf{x}) = \mathcal{N}(\mathbf{x}; \hat{\mu}_k, \hat{\Sigma}_k)$$

- But when the dimensionality of \mathbf{x} gets large or there is high correlation, estimation of $\hat{\Sigma}_k$ can be poor
- If we force $\hat{\Sigma}_k$ to be *diagonal* then the densities are product of univariate Gaussians (called Gaussian Naive Bayes)

$$\hat{f}_k(\mathbf{x}) = \prod_{j=1}^p \mathcal{N}(x_j; \mu_{kj}, \frac{\sigma_{kj}}{\sigma_{kj}})$$

- Even if the data are not independent, this may give better estimates by reducing the variance (at the expense of a bit of bias)
- This is a special case of QDA, where we restrict the off-diagonal terms in the variance-covariance to be 0.

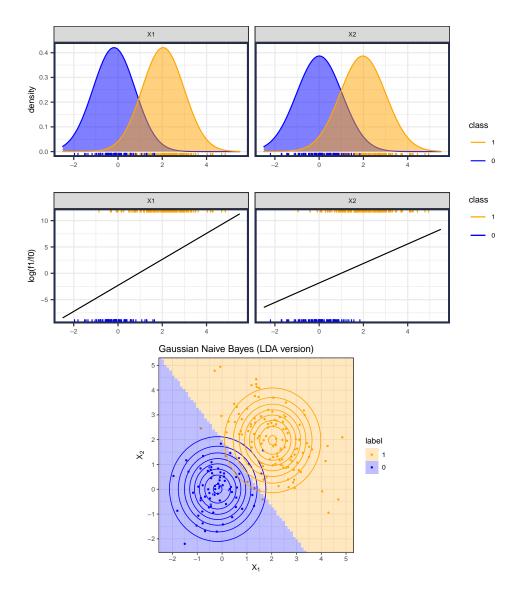
class	predictor	mu	sd	density
0	X1	-0.18	0.73	N(mu = -0.18, sd = 0.73)
0	X2	0.01	0.81	N(mu = 0.01, sd = 0.81)
1	X1	2.04	1.06	N(mu = 2.04, sd = 1.06)
1	X2	1.97	1.15	N(mu = 1.97, sd = 1.15)



• A simpler model (less complexity/edf) forces a common standard deviation for all class (special case of LDA)

$$\hat{f}_k(\mathbf{x}) = \prod_{j=1}^p \mathcal{N}(x_j; \mu_{kj}, \sigma_j)$$

class	predictor	mu	sd
0	X1	-0.18	0.95
0	X2	0.01	1.03
1	X1	2.04	0.95
1	X2	1.97	1.03



5.2 Kernel Naive Bayes

In kernel density Naive Bayes, use Kernel Density Estimation (KDE) to estimate each component density:

$$\hat{f}_{kj}(x_j) = \frac{1}{n_k} \sum_{i:g_i = k} K(x_j - x_{ij}; h_{kj})$$

with bandwidth parameter h_{kj} .

The density ratio becomes

$$\frac{\hat{f}_{1j}(x_j)}{\hat{f}_{0j}(x_j)} = \frac{\frac{1}{n_1}\sum_{i:g_i=1}K(x_j-x_{ij};h_{1j})}{\frac{1}{n_0}\sum_{i:g_i=0}K(x_j-x_{ij};h_{0j})}$$

• for less complex models, use same bandwidth parameter for each class.

Note: this gives a different solution than using KDE with a *product kernel*! (which is not a naive bayes model)

$$\hat{f}_k(\mathbf{x}) = \frac{1}{n_k} \sum_{i:q_i=k} \prod_{j=1}^p K(x_j - x_{ij}; h_{kj})$$

6 Connections: Generalized Additive Models (GAM)

It turns out that there is a close connection between Logistic Regression, Naive Bayes, and LDA. To help see this, notice that all three methods can be written:

$$\gamma(x) = \log\left(\frac{\pi}{1-\pi}\right) + \log\left(\frac{f_1(x)}{f_0(x)}\right)$$
$$= \alpha_0 + \sum_{j=1}^p \alpha_j S_j$$

• Logistic Regression

$$\hat{\alpha}_0 = \hat{\beta}_0$$

$$\hat{\alpha}_j = \hat{\beta}_j$$

$$\hat{S}_j = x_j$$

• LDA

$$\hat{\alpha}_0 = \log \frac{\hat{\pi}}{1 - \hat{\pi}} - \frac{1}{2} (\hat{\mu}_1 + \hat{\mu}_0)^{\mathsf{T}} \hat{\Sigma}^{-1} (\hat{\mu}_1 - \hat{\mu}_0)$$

$$\hat{\alpha}_j = \hat{\Sigma}^{-1} (\hat{\mu}_1 - \hat{\mu}_0)$$

$$\hat{S}_j = x_j$$

Naive Bayes

$$\hat{\alpha}_0 = \log \frac{\hat{\pi}}{1 - \hat{\pi}}$$

$$\hat{\alpha}_j = 1$$

$$\hat{S}_j = \log \frac{\hat{f}_{1j}(x_j)}{\hat{f}_{0j}(x_j)}$$

• Generalized Additive Models (GAM)

- GAM models are made to directly estimate models of this form.

$$\hat{\gamma}(x) = \hat{\alpha} + \sum_{j=1}^{p} \hat{g}_j(x_j)$$

- $g_j(x_j)$ is non-linear (usually based on penalized splines)
- In **R**, the mgcv package is worth becoming familiar with to implement GAM.
- See ESL 9.1 for more details