Linear Methods for Classification

TrungTin Nguyen

STATIFY team, Inria centre at the University Grenoble Alpes, France

Statistical Analysis and Document Mining

Complementary Course, Master of Applied Mathematics in Grenoble

Outline

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Previous episode: Nearest-neighbour methods

- We are given a **training dataset** $\mathcal{D} \equiv \{(\mathbf{x}_n, y_n)\}_{n\in[N]}$, $y_{[N]} \in \mathcal{C} \subsetneq \mathbb{N}$, i.i.d. sampled from **the true (but unknown) joint PDF** of $(\mathbf{X}, Y)$.

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- How to model relationship between $p_c(\mathbf{X}) = \mathbb{P}(Y = c|\mathbf{X})$, $c \in \mathcal{C}$, and $\mathbf{X}$?
- K-Nearest-neighbours (kNN) approximate the probability that Y belongs to a particular category instead Y,

$$\mathbb{P}(Y = c|\mathbf{X} = \mathbf{x}) \approx \frac{1}{K} \sum_{\mathbf{x}_n \in \mathcal{N}_K(\mathbf{x})} \mathbb{1}_{y=c}(y_n).$$

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- The hyper-parameter K usually chosen via cross-validation.

It works well in low dimensions, but suffers from the curse of dimensionality. Verified in CC5!

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- How to model relationship between $p_c(\mathbf{X}) = \mathbb{P}(Y = c|\mathbf{X})$, $c \in \mathcal{C}$, and $\mathbf{X}$?
- Which is suitable for high-dimensional data: Discriminative approaches (CM5) or Generative approaches (CM6).
  1. K-nearest neighbors (K-NN) (CM5),
  2. Logistic Regression (CM5),
  3. Linear Discriminant Analysis (CM6),
  4. Naive Bayes classifier (CM6).

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   - Previous episode: multiple impact of high-dimensionality on statistics
   - Multinomial logistic regression
   - Baseline and softmax coding in multinomial linear regression
2. Generalized Linear Models
   - Previous episode: linear regression for bikeshare data set
   - Bikeshare data: Poisson regression
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For more details, see [Giraud, 2021, Chapter 1].

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- Multiple logistic regression takes the form $p_2(\mathbf{X}) = 1 - p_1(\mathbf{X})$, and models the probability that Y belongs to a particular category instead Y,

$$\log\left(\frac{p_1(\mathbf{X})}{1 - p_1(\mathbf{X})}\right) = \beta_0 + \sum_{p=1}^{P} \beta_p X_p, \text{ or } p_1(\mathbf{X}) = \frac{\exp(\beta_0 + \sum_{p=1}^{P} \beta_p X_p)}{1 + \exp(\beta_0 + \sum_{p=1}^{P} \beta_p X_p)}.$$

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- **Training error:** using non-linear LS or maximum likelihood estimation (MLE), we obtain $\widehat{\beta}$ and $\widehat{r}_{\mathcal{D}}(\mathbf{x}_n) = \operatorname{argmax}_{c\in\mathcal{C}} p_c(\mathbf{x}_n)$ such that $\forall n \in [N]$,

$$y_n \approx \widehat{r}_{\mathcal{D}}(\mathbf{x}_n), \text{ or equivalent, } \mathcal{L}(\widehat{r}_{\mathcal{D}}, \mathcal{D}) \equiv \frac{1}{N}\sum_{n=1}^{N} \mathbb{1}\left[y_n \neq \widehat{r}_{\mathcal{D}}(\mathbf{x}_n)\right] \approx 0. \quad (1)$$

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Test (generalization) error: for any **new sample** $(\mathbf{x}^*, y^*)$, how we guarantee

$$y^* \approx \widehat{r}_{\mathcal{D}}(\mathbf{x}^*), \text{ or equivalent, } \mathcal{L}(\widehat{r}_{\mathcal{D}}) \equiv \mathbb{E}_{\mathbf{X},Y}\left[\mathbb{1}\left(Y \neq \widehat{r}_{\mathcal{D}}(\mathbf{X})\right)\right] \approx 0? \quad (2)$$

Multinomial logistic regression

- We are given a **training dataset** $\mathcal{D} \equiv \{(\mathbf{x}_n, y_n)\}_{n\in[N]}$, $y_{[N]} \in \mathcal{C} \equiv [K]$, i.i.d. sampled from **the true (but unknown) joint PDF** of $(\mathbf{X}, Y)$.

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- How to model relationship between $p_k(\mathbf{X}) = \mathbb{P}(Y = k|\mathbf{X})$, $k \in [K]$, and $\mathbf{X}$?
- Multinomial logistic regression (LR) takes the form $p_K(\mathbf{X}) = 1 - \sum_{k=1}^{K-1} p_k(\mathbf{X})$, and models the probability that Y belongs to a particular category instead of the value of Y as follows:

$$\log\left(\frac{p_k(\mathbf{X})}{p_K(\mathbf{X})}\right) = \beta_{k0} + \sum_{p=1}^{P} \beta_{kp} x_p, \text{ or equivalent,}$$

$$p_k(\mathbf{X}) = \frac{\exp(\beta_{k0} + \sum_{p=1}^{P} \beta_{kp} x_p)}{1 + \sum_{l=1}^{K-1} \exp(\beta_{l0} + \sum_{p=1}^{P} \beta_{lp} X_p)}.$$

Here, we first select a single class to serve as the baseline; without loss of generality, we select the Kth class for this role. It holds that

$$p_K(\mathbf{X}) = \frac{1}{1 + \sum_{l=1}^{K-1} \exp(\beta_{l0} + \sum_{p=1}^{P} \beta_{lp} X_p)}. \tag{3}$$

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Multinomial LR: baseline and softmax coding

- Log-odds or logit transformations using baseline coding: $p_K(\mathbf{X}) = 1 - \sum_{k=1}^{K-1} p_k(\mathbf{X}) =?$,

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- Log-odds using softmax coding takes the form

$$\log\left(\frac{p_k(\mathbf{X})}{p_k'(\mathbf{X})}\right) = (\beta_{k0} - \beta_{k'0}) + \sum_{p=1}^{P} \left(\beta_{kp} - \beta_{k'p}\right) X_p, \text{ or equivalent,}$$

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In multinomial LR, the fitted values, log odds between any pair of classes, and other key ~~model outputs will remain the same, regardless of coding!~~

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Bikeshare data set: motivation example

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Predicting bikers using the covariates mnth (month of the year), hr (hour of the day, from 0 to 23), workingday (an indicator variable that equals 1 if it is neither a weekend nor a holiday), temp (the normalized temperature, in Celsius), and weathersit (a qualitative variable that takes on one of four possible values: clear; misty or cloudy; light rain or light snow; or heavy rain or heavy snow.)

```
> head(Bikeshare)
  season mnth day hr holiday weekday workingday   weathersit temp  atemp  hum windspeed casual registered bikers
1      1  Jan   1  0       0       6          0        clear 0.24 0.2879 0.81    0.0000      3         13     16
2      1  Jan   1  1       0       6          0        clear 0.22 0.2727 0.80    0.0000      8         32     40
3      1  Jan   1  2       0       6          0        clear 0.22 0.2727 0.80    0.0000      5         27     32
4      1  Jan   1  3       0       6          0        clear 0.24 0.2879 0.75    0.0000      3         10     13
5      1  Jan   1  4       0       6          0        clear 0.24 0.2879 0.75    0.0000      0          1      1
6      1  Jan   1  5       0       6          0 cloudy/misty 0.24 0.2576 0.75    0.0896      0          1      1
```

```
> mod.lm2 <- lm(
+     bikers ~ mnth + hr + workingday + temp + weathersit,
+     data = Bikeshare
+   )
> summary(mod.lm2)

Call:
lm(formula = bikers ~ mnth + hr + workingday + temp + weathersit,
    data = Bikeshare)

Residuals:
    Min      1Q  Median      3Q     Max
-299.00  -45.70   -6.23   41.08  425.29

Coefficients:
                          Estimate Std. Error t value Pr(>|t|)
(Intercept)                73.5974     5.1322  14.340  < 2e-16 ***
mnth1                     -46.0871     4.0855 -11.281  < 2e-16 ***
mnth2                     -39.2419     3.5391 -11.088  < 2e-16 ***
mnth3                     -29.5357     3.1552  -9.361  < 2e-16 ***
mnth4                      -4.6622     2.7406  -1.701  0.08895 .
mnth5                      26.4700     2.8508   9.285  < 2e-16 ***
mnth6                      21.7317     3.4651   6.272 3.75e-10 ***
mnth7                      -0.7626     3.9084  -0.195  0.84530
mnth8                       7.1560     3.5347   2.024  0.04295 *
mnth9                      20.5912     3.0456   6.761 1.46e-11 ***
mnth10                     29.7472     2.6995  11.019  < 2e-16 ***
mnth11                     14.2229     2.8604   4.972 6.74e-07 ***
```

```
mnth11                  14.2229     2.8604   4.972 6.74e-07 ***
hr1                    -96.1420     3.9554 -24.307  < 2e-16 ***
hr2                   -110.7213     3.9662 -27.916  < 2e-16 ***
hr3                   -117.7212     4.0165 -29.310  < 2e-16 ***
hr4                   -127.2828     4.0808 -31.191  < 2e-16 ***
hr5                   -133.0495     4.1168 -32.319  < 2e-16 ***
hr6                   -120.2775     4.0370 -29.794  < 2e-16 ***
hr7                    -75.5424     3.9916 -18.925  < 2e-16 ***
hr8                     23.9511     3.9686   6.035 1.65e-09 ***
hr9                    127.5199     3.9500  32.284  < 2e-16 ***
hr10                    24.4399     3.9360   6.209 5.57e-10 ***
hr11                   -12.3407     3.9361  -3.135  0.00172 **
hr12                     9.2814     3.9447   2.353  0.01865 *
hr13                    41.1417     3.9571  10.397  < 2e-16 ***
hr14                    39.8939     3.9750  10.036  < 2e-16 ***
hr15                    30.4940     3.9910   7.641 2.39e-14 ***
hr16                    35.9445     3.9949   8.998  < 2e-16 ***
hr17                    82.3786     3.9883  20.655  < 2e-16 ***
hr18                   200.1249     3.9638  50.488  < 2e-16 ***
hr19                   173.2989     3.9561  43.806  < 2e-16 ***
hr20                    90.1138     3.9400  22.872  < 2e-16 ***
hr21                    29.4071     3.9362   7.471 8.74e-14 ***
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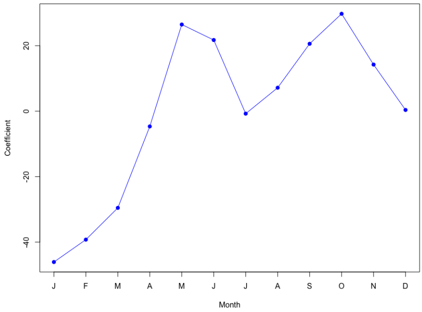

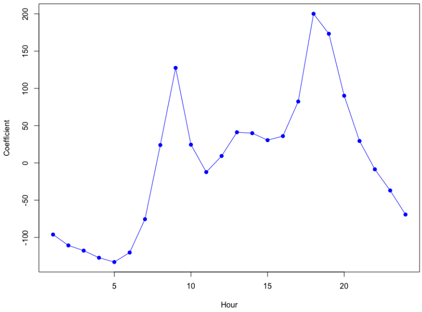

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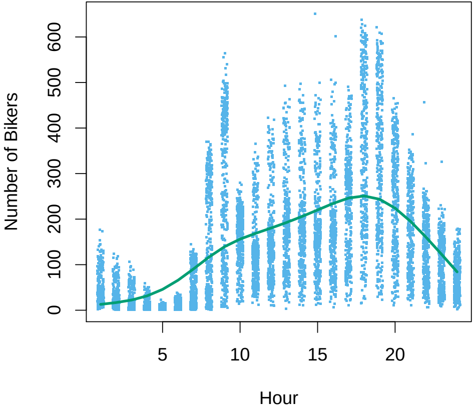

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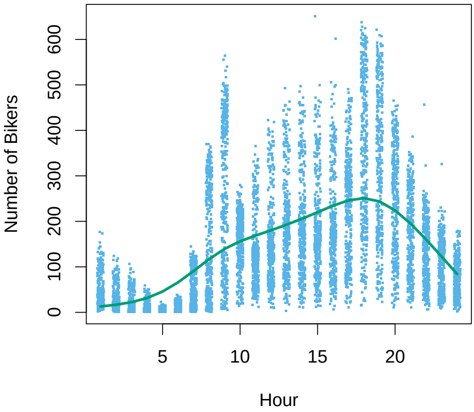

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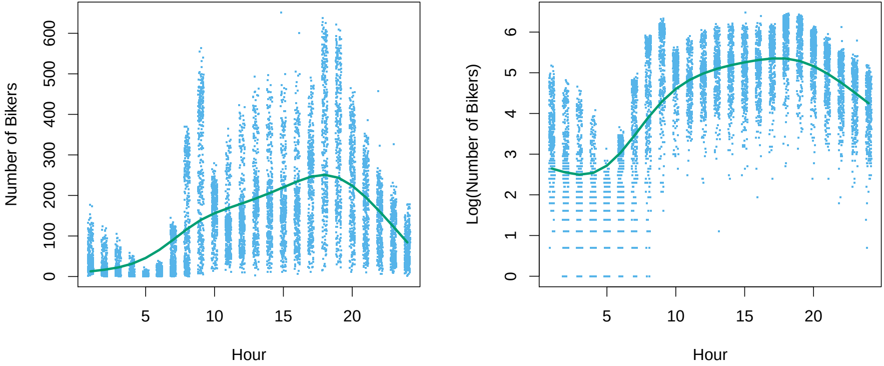
1. **9.6% of the fitted values** in the Bikeshare data set are **negative**: that is, the linear regression model predicts a negative number of users during 9.6% of the hours in the data set.
2. Since ϵ is a continuous-valued error term, response Y is necessarily continuous-valued (quantitative) but the response bikers is integer-valued.

3. The mean-variance relationship is a major violation of the assumptions of a linear model, which state that $Y = \beta_0 + \sum_{p=1}^{P} X_p \beta_p + \epsilon$, where ϵ is a mean-zero error term with variance σ^2 that is constant, and not a function of the covariates. For the most part, as the mean number of bikers increases, so does the variance in the number of bikers!



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- Transforming the mean of response $\mathbb{E}[Y]$ as in the logistic regression!

Outline

Poisson Regression

- Definition of Poisson distribution:

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$$\mathbb{P}(Y = k) = \frac{e^{\lambda}\lambda^k}{k!} \text{ for } k = 0, 1, 2, \ldots, \lambda > 0. \tag{4}$$

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- MLE approach: we want to maximize MLE

$$l(\beta_0, \beta_1, \ldots, \beta_P) = \prod_{n=1}^{N} \frac{e^{-\lambda(x_n)}\lambda(x_n)^{y_n}}{y_n!}, \quad \lambda(x_n) = \exp(\beta_0 + \sum_{p=1}^{P} x_{np}\beta_p). \tag{6}$$

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   - Previous episode: nearest-neighbour methods
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   - Multinomial logistic regression
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2. Generalized Linear Models
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   - Bikeshare data: linear regression and Poisson regression
   - Generalized linear models
3. A Mathematical Comparison of Classification Methods
   - LDA and multinomial LR
   - LDA, QDA, and naive Bayes

```
> mod.lm2 <- lm(
+     bikers ~ mnth + hr + workingday + temp + weathersit,
+     data = Bikeshare
+   )
> summary(mod.lm2)

Call:
lm(formula = bikers ~ mnth + hr + workingday + temp + weathersit,
    data = Bikeshare)

Residuals:
    Min      1Q  Median      3Q     Max 
-299.00  -45.70   -6.23   41.08  425.29 

Coefficients:
                           Estimate Std. Error t value Pr(>|t|)    
(Intercept)                 73.5974     5.1322  14.340  < 2e-16 ***
mnth1                      -46.0871     4.0855 -11.281  < 2e-16 ***
mnth2                      -39.2419     3.5391 -11.088  < 2e-16 ***
mnth3                      -29.5357     3.1552  -9.361  < 2e-16 ***
mnth4                       -4.6622     2.7406  -1.701  0.08895 .  
mnth5                       26.4700     2.8508   9.285  < 2e-16 ***
mnth6                       21.7317     3.4651   6.272 3.75e-10 ***
mnth7                       -0.7626     3.9084  -0.195  0.84530    
mnth8                        7.1560     3.5347   2.024  0.04295 *  
mnth9                       20.5912     3.0456   6.761 1.46e-11 ***
mnth10                      29.7472     2.6995  11.019  < 2e-16 ***
mnth11                      14.2229     2.8604   4.972 6.74e-07 ***
```

```
> mod.pois <- glm(
+     bikers ~ mnth + hr + workingday + temp + weathersit,
+     data = Bikeshare, family = poisson
+   )
> summary(mod.pois)

Call:
glm(formula = bikers ~ mnth + hr + workingday + temp + weathersit,
    family = poisson, data = Bikeshare)

Deviance Residuals:
     Min        1Q    Median        3Q       Max
-20.7574   -3.3441   -0.6549    2.6999   21.9628

Coefficients:
                           Estimate Std. Error  z value Pr(>|z|)
(Intercept)                4.118245   0.006021  683.964  < 2e-16 ***
mnth1                     -0.670170   0.005907 -113.445  < 2e-16 ***
mnth2                     -0.444124   0.004860  -91.379  < 2e-16 ***
mnth3                     -0.293733   0.004144  -70.886  < 2e-16 ***
mnth4                      0.021523   0.003125    6.888 5.66e-12 ***
mnth5                      0.240471   0.002916   82.462  < 2e-16 ***
mnth6                      0.223235   0.003554   62.818  < 2e-16 ***
mnth7                      0.103617   0.004125   25.121  < 2e-16 ***
mnth8                      0.151171   0.003662   41.281  < 2e-16 ***
mnth9                      0.233493   0.003102   75.281  < 2e-16 ***
mnth10                     0.267573   0.002785   96.091  < 2e-16 ***
mnth11                     0.150264   0.003180   47.248  < 2e-16 ***
```

```
mnth11                      14.2229     2.8604   4.972 6.74e-07 ***
hr1                        -96.1420     3.9554 -24.307  < 2e-16 ***
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hr22                        -8.5883     3.9332  -2.184  0.02902 *
hr23                       -37.0194     3.9344  -9.409  < 2e-16 ***
workingday                   1.2696     1.7845   0.711  0.47681
temp                       157.2094    10.2612  15.321  < 2e-16 ***
weathersitcloudy/misty     -12.8903     1.9643  -6.562 5.60e-11 ***
weathersitlight rain/snow  -66.4944     2.9652 -22.425  < 2e-16 ***
```

```
hr11                       0.336852   0.004720   71.372  < 2e-16 ***
hr12                       0.494121   0.004392  112.494  < 2e-16 ***
hr13                       0.679642   0.004069  167.040  < 2e-16 ***
hr14                       0.673565   0.004089  164.722  < 2e-16 ***
hr15                       0.624910   0.004178  149.570  < 2e-16 ***
hr16                       0.653763   0.004132  158.205  < 2e-16 ***
hr17                       0.874301   0.003784  231.040  < 2e-16 ***
hr18                       1.294635   0.003254  397.848  < 2e-16 ***
hr19                       1.212281   0.003321  365.084  < 2e-16 ***
hr20                       0.914022   0.003700  247.065  < 2e-16 ***
hr21                       0.616201   0.004191  147.045  < 2e-16 ***
hr22                       0.364181   0.004659   78.173  < 2e-16 ***
hr23                       0.117493   0.005225   22.488  < 2e-16 ***
workingday                 0.014665   0.001955    7.502 6.27e-14 ***
temp                       0.785292   0.011475   68.434  < 2e-16 ***
weathersitcloudy/misty    -0.075231   0.002179  -34.528  < 2e-16 ***
weathersitlight rain/snow -0.575800   0.004058 -141.905  < 2e-16 ***
weathersitheavy rain/snow -0.926287   0.166782   -5.554 2.79e-08 ***
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1

(Dispersion parameter for poisson family taken to be 1)

    Null deviance: 1052921  on 8644  degrees of freedom
Residual deviance:  228041  on 8605  degrees of freedom
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Number of Fisher Scoring iterations: 5
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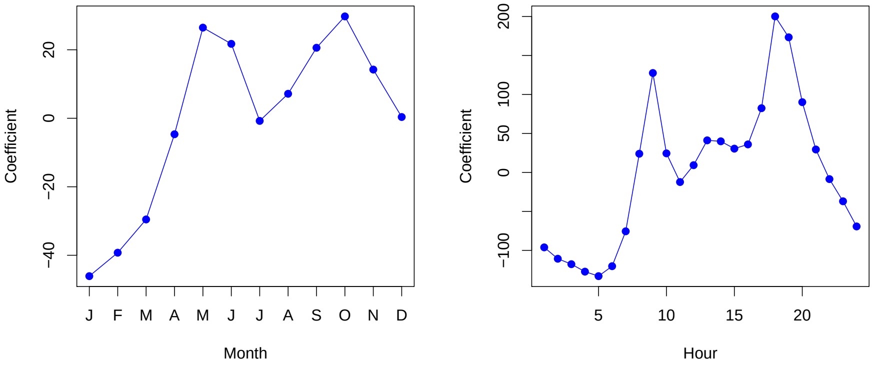

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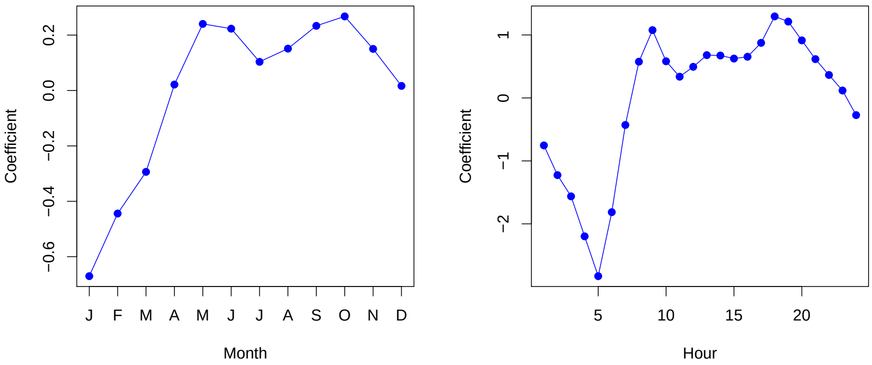

A Poisson regression model was fit to predict bikers in the Bikeshare data set. Left: The coefficients associated with the month of the year. Bike usage is highest in the spring and fall, and lowest in the winter. Right: The coefficients associated with the hour of the day. Bike usage is highest during peak commute times, and lowest overnight [James et al., 2021, Figure 4.15]

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2. **Mean-variance relationship:** in Poisson regression, we implicitly assume that **mean bike usage in a given hour equals the variance of bike usage during that hour** while a constant variance in linear regression model.
3. **Nonnegative fitted values:** there are no negative predictions using the Poisson regression model.

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3. Poisson regression $\mathbb{E}\left[Y|X_{[P]}\right] = \lambda(X_{[P]}) = e^{\beta_0 + \sum_{p=1}^{P} \beta_p X_p}$.

Generalized linear models

Recall that conditional on $X_{[P]} \equiv (X_1, \ldots, X_P)$, Y belongs to a certain family of distributions: Gaussian or normal distribution for linear regression, Bernoulli distribution for logistic regression and Poisson distribution for Poisson regression. What is the common thing?

$Y \in$ exponential family (including Gaussian, Bernoulli & Poisson).

Each approach models the mean of Y as a function of the predictors.

1. Linear regression $\mathbb{E}\left[Y|X_{[P]}\right] = \beta_0 + \sum_{p=1}^{P} \beta_p X_p$.
2. Logistic regression $\mathbb{E}\left[Y|X_{[P]}\right] = \mathbb{P}(Y = 1|X_{[P]}) = \frac{e^{\beta_0 + \sum_{p=1}^{P} \beta_p X_p}}{1 + e^{\beta_0 + \sum_{p=1}^{P} \beta_p X_p}}$.
3. Poisson regression $\mathbb{E}\left[Y|X_{[P]}\right] = \lambda(X_{[P]}) = e^{\beta_0 + \sum_{p=1}^{P} \beta_p X_p}$.

Using a link function η such that $\eta\left(\mathbb{E}\left[Y|X_{[P]}\right]\right) = \beta_0 + \sum_{p=1}^{P} \beta_p X_p$.

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HOW.

Generalized linear models

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HOW. $\eta(\mu) = \mu$, $\eta(\mu) = \log(\mu/(1-\mu))$, $\eta(\mu) = \log(\mu)$.

Outline

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Log odds of posterior probabilities with normal assumptions

We now make an analytical (or mathematical) comparison between Linear discriminant analysis (LDA), Quadratic discriminant analysis (QDA), naive Bayes and multinomial LR, see [James et al., 2021] for more details.

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Log odds of posterior probabilities with normal assumptions

We now make an analytical (or mathematical) comparison between Linear discriminant analysis (LDA), Quadratic discriminant analysis (QDA), naive Bayes and multinomial LR, see [James et al., 2021] for more details.

- We consider these approaches in a setting with K classes, so that we assign an observation to the class that maximizes $\mathbb{P}(Y = k|\mathbf{X} = \mathbf{x})$.
- Equivalently, via considering K as the baseline class, Bayes' Theorem and $\mathbf{X}|Y = k \sim \mathcal{N}(\boldsymbol{\mu}_k, \Sigma)$, we aim to maximize

$$\log\left(\frac{\mathbb{P}(Y = k|\mathbf{X} = \mathbf{x})}{\mathbb{P}(Y = K|\mathbf{X} = \mathbf{x})}\right) = a_k + \sum_{p=1}^{P} b_{kp}x_p \quad (7)$$

- **What are the value of a_k and b_{kp}?**

Log odds of posteriors in LDA and multinomial LR

In LDA, we maximize the following log odds of the posterior:

$$
\begin{aligned}
\log\left(\frac{\mathbb{P}(Y=k|\mathbf{X}=\mathbf{x})}{\mathbb{P}(Y=K|\mathbf{X}=\mathbf{x})}\right) &= \log\left(\frac{\mathbb{P}(Y=k)\mathbb{P}(\mathbf{X}=\mathbf{x}|Y=k)}{\mathbb{P}(Y=K)\mathbb{P}(\mathbf{X}=\mathbf{x}|Y=K)}\right) \\
&= \log\left(\frac{\pi_k \exp(-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu}_k)^\top \boldsymbol{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu}_k))}{\pi_K \exp(-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu}_K)^\top \boldsymbol{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu}_K))}\right) \\
&= \log\left(\frac{\pi_k}{\pi_K}\right) - \frac{1}{2}(\mathbf{x}-\boldsymbol{\mu}_k)^\top \boldsymbol{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu}_k) + \frac{1}{2}(\mathbf{x}-\boldsymbol{\mu}_K)^\top \boldsymbol{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu}_K) \\
&= \underbrace{\log\left(\frac{\pi_k}{\pi_K}\right) - \frac{1}{2}(\boldsymbol{\mu}_k+\boldsymbol{\mu}_K)^\top \boldsymbol{\Sigma}^{-1}(\boldsymbol{\mu}_k-\boldsymbol{\mu}_K)}_{\equiv a_k} + \mathbf{x}^\top \underbrace{\boldsymbol{\Sigma}^{-1}(\boldsymbol{\mu}_k-\boldsymbol{\mu}_K)}_{\equiv \boldsymbol{b}_k} \\
&= a_k + \sum_{p=1}^{P} b_{kp} x_p, \ \text{linear in } \mathbf{x}. \qquad (8)
\end{aligned}
$$

Log odds of posteriors in LDA and multinomial LR

In LDA, we maximize the following log odds of the posterior:

$$\begin{aligned}
\log\left(\frac{\mathbb{P}(Y=k|\mathbf{X}=\mathbf{x})}{\mathbb{P}(Y=K|\mathbf{X}=\mathbf{x})}\right) &= \log\left(\frac{\mathbb{P}(Y=k)\mathbb{P}(\mathbf{X}=\mathbf{x}|Y=k)}{\mathbb{P}(Y=K)\mathbb{P}(\mathbf{X}=\mathbf{x}|Y=K)}\right)\\
&= \log\left(\frac{\pi_k \exp(-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu}_k)^\top\boldsymbol{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu}_k))}{\pi_K \exp(-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu}_K)^\top\boldsymbol{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu}_K))}\right)\\
&= \log\left(\frac{\pi_k}{\pi_K}\right) - \frac{1}{2}(\mathbf{x}-\boldsymbol{\mu}_k)^\top\boldsymbol{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu}_k) + \frac{1}{2}(\mathbf{x}-\boldsymbol{\mu}_K)^\top\boldsymbol{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu}_K)\\
&= \underbrace{\log\left(\frac{\pi_k}{\pi_K}\right) - \frac{1}{2}(\boldsymbol{\mu}_k+\boldsymbol{\mu}_K)^\top\boldsymbol{\Sigma}^{-1}(\boldsymbol{\mu}_k-\boldsymbol{\mu}_K)}_{\equiv a_k} + \mathbf{x}^\top \underbrace{\boldsymbol{\Sigma}^{-1}(\boldsymbol{\mu}_k-\boldsymbol{\mu}_K)}_{\equiv \boldsymbol{b}_k}\\
&= a_k + \sum_{p=1}^{P} b_{kp}x_p, \text{ linear in } \mathbf{x}. \qquad (8)
\end{aligned}$$

Recall that for multinomial LR:

$$\log\left(\frac{\mathbb{P}(Y=k|\mathbf{X}=\mathbf{x})}{\mathbb{P}(Y=K|\mathbf{X}=\mathbf{x})}\right) = \beta_{k0} + \sum_{p=1}^{P}\beta_{kp}x_p, \text{ linear in } \mathbf{x}.$$

Log odds of posteriors in LDA and multinomial LR

In LDA, we maximize the following log odds of the posterior:

$$
\begin{aligned}
\log\left(\frac{\mathbb{P}(Y=k|\mathbf{X}=\mathbf{x})}{\mathbb{P}(Y=K|\mathbf{X}=\mathbf{x})}\right) &= \log\left(\frac{\mathbb{P}(Y=k)\mathbb{P}(\mathbf{X}=\mathbf{x}|Y=k)}{\mathbb{P}(Y=K)\mathbb{P}(\mathbf{X}=\mathbf{x}|Y=K)}\right) \\
&= \log\left(\frac{\pi_k \exp(-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu}_k)^\top \boldsymbol{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu}_k))}{\pi_K \exp(-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu}_K)^\top \boldsymbol{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu}_K))}\right) \\
&= \log\left(\frac{\pi_k}{\pi_K}\right) - \frac{1}{2}(\mathbf{x}-\boldsymbol{\mu}_k)^\top \boldsymbol{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu}_k) + \frac{1}{2}(\mathbf{x}-\boldsymbol{\mu}_K)^\top \boldsymbol{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu}_K) \\
&= \underbrace{\log\left(\frac{\pi_k}{\pi_K}\right) - \frac{1}{2}(\boldsymbol{\mu}_k+\boldsymbol{\mu}_K)^\top \boldsymbol{\Sigma}^{-1}(\boldsymbol{\mu}_k-\boldsymbol{\mu}_K)}_{\equiv a_k} + \mathbf{x}^\top \underbrace{\boldsymbol{\Sigma}^{-1}(\boldsymbol{\mu}_k-\boldsymbol{\mu}_K)}_{\equiv \boldsymbol{b}_k} \\
&= a_k + \sum_{p=1}^{P} b_{kp}x_p, \ \text{linear in } \mathbf{x}. \qquad (8)
\end{aligned}
$$

Recall that for multinomial LR:

$$
\log\left(\frac{\mathbb{P}(Y=k|\mathbf{X}=\mathbf{x})}{\mathbb{P}(Y=K|\mathbf{X}=\mathbf{x})}\right) = \beta_{k0} + \sum_{p=1}^{P} \beta_{kp}x_p, \ \text{linear in } \mathbf{x}.
$$

Both LDA and multinomial LR assume that the log odds of the posterior probabilities is linear in $\mathbf{x}$.

Outline

Log odds of posterior probabilities in QDA and LDA

In QDA, $\mathbf{X}|Y = k \sim \mathcal{N}(\boldsymbol{\mu}_k, \Sigma_k)$ we maximize the following log odds of the posterior:

$$\begin{aligned}
\log\left(\frac{\mathbb{P}(Y = k|\mathbf{X} = \mathbf{x})}{\mathbb{P}(Y = K|\mathbf{X} = \mathbf{x})}\right) &= \log\left(\frac{\mathbb{P}(Y = k)\mathbb{P}(\mathbf{X} = \mathbf{x}|Y = k)}{\mathbb{P}(Y = K)\mathbb{P}(\mathbf{X} = \mathbf{x}|Y = K)}\right) \\
&= \log\left(\frac{\pi_k \exp(-\frac{1}{2}(\mathbf{x} - \boldsymbol{\mu}_k)^\top \boldsymbol{\Sigma}_k^{-1}(\mathbf{x} - \boldsymbol{\mu}_k))}{\pi_K \exp(-\frac{1}{2}(\mathbf{x} - \boldsymbol{\mu}_K)^\top \boldsymbol{\Sigma}_K^{-1}(\mathbf{x} - \boldsymbol{\mu}_K))}\right) \\
&= \log\left(\frac{\pi_k}{\pi_K}\right) - \frac{1}{2}(\mathbf{x} - \boldsymbol{\mu}_k)^\top \boldsymbol{\Sigma}_k^{-1}(\mathbf{x} - \boldsymbol{\mu}_k) + \frac{1}{2}(\mathbf{x} - \boldsymbol{\mu}_K)^\top \boldsymbol{\Sigma}_K^{-1}(\mathbf{x} - \boldsymbol{\mu}_K) \\
&= a_k + \sum_{p=1}^{P} b_{kp}x_p + \sum_{p=1}^{P}\sum_{q=1}^{Q} c_{kpq}x_px_q, \ \text{quadratic in } \mathbf{x}, \qquad (9)
\end{aligned}$$

Log odds of posterior probabilities in QDA and LDA

In QDA, $\mathbf{X}|Y = k \sim \mathcal{N}(\boldsymbol{\mu}_k, \Sigma_k)$ we maximize the following log odds of the posterior:

$$
\begin{aligned}
\log\left(\frac{\mathbb{P}(Y=k|\mathbf{X}=\mathbf{x})}{\mathbb{P}(Y=K|\mathbf{X}=\mathbf{x})}\right) &= \log\left(\frac{\mathbb{P}(Y=k)\mathbb{P}(\mathbf{X}=\mathbf{x}|Y=k)}{\mathbb{P}(Y=K)\mathbb{P}(\mathbf{X}=\mathbf{x}|Y=K)}\right) \\
&= \log\left(\frac{\pi_k \exp(-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu}_k)^\top \boldsymbol{\Sigma}_k^{-1}(\mathbf{x}-\boldsymbol{\mu}_k))}{\pi_K \exp(-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu}_K)^\top \boldsymbol{\Sigma}_K^{-1}(\mathbf{x}-\boldsymbol{\mu}_K))}\right) \\
&= \log\left(\frac{\pi_k}{\pi_K}\right) - \frac{1}{2}(\mathbf{x}-\boldsymbol{\mu}_k)^\top \boldsymbol{\Sigma}_k^{-1}(\mathbf{x}-\boldsymbol{\mu}_k) + \frac{1}{2}(\mathbf{x}-\boldsymbol{\mu}_K)^\top \boldsymbol{\Sigma}_K^{-1}(\mathbf{x}-\boldsymbol{\mu}_K) \\
&= a_k + \sum_{p=1}^{P} b_{kp}x_p + \sum_{p=1}^{P}\sum_{q=1}^{Q} c_{kpq}x_p x_q, \text{ quadratic in } \mathbf{x}, \qquad (9)
\end{aligned}
$$

where a_k, b_{kp}, c_{kpq} are functions of $\pi_k, \pi_K, \boldsymbol{\mu}_k, \boldsymbol{\mu}_K, \boldsymbol{\Sigma}_k, \boldsymbol{\Sigma}_K$.

Log odds of posterior probabilities in QDA and LDA

In QDA, $\mathbf{X}|Y = k \sim \mathcal{N}(\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)$ we maximize the following log odds of the posterior:

$$
\begin{aligned}
\log\left(\frac{\mathbb{P}(Y=k|\mathbf{X}=\mathbf{x})}{\mathbb{P}(Y=K|\mathbf{X}=\mathbf{x})}\right) &= \log\left(\frac{\mathbb{P}(Y=k)\mathbb{P}(\mathbf{X}=\mathbf{x}|Y=k)}{\mathbb{P}(Y=K)\mathbb{P}(\mathbf{X}=\mathbf{x}|Y=K)}\right) \\
&= \log\left(\frac{\pi_k \exp(-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu}_k)^\top \boldsymbol{\Sigma}_k^{-1}(\mathbf{x}-\boldsymbol{\mu}_k))}{\pi_K \exp(-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu}_K)^\top \boldsymbol{\Sigma}_K^{-1}(\mathbf{x}-\boldsymbol{\mu}_K))}\right) \\
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&= a_k + \sum_{p=1}^{P} b_{kp}x_p + \sum_{p=1}^{P}\sum_{q=1}^{Q} c_{kpq}x_p x_q, \text{ quadratic in } \mathbf{x}, \qquad (9)
\end{aligned}
$$

where a_k, b_{kp}, c_{kpq} are functions of $\pi_k, \pi_K, \boldsymbol{\mu}_k, \boldsymbol{\mu}_K, \boldsymbol{\Sigma}_k, \boldsymbol{\Sigma}_K$. Recall that for LDA:

$$
\log\left(\frac{\mathbb{P}(Y=k|\mathbf{X}=\mathbf{x})}{\mathbb{P}(Y=K|\mathbf{X}=\mathbf{x})}\right) = a_k + \sum_{p=1}^{P} b_{kp}x_p, \text{ linear in } \mathbf{x}.
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In QDA, $\mathbf{X}|Y = k \sim \mathcal{N}(\boldsymbol{\mu}_k, \Sigma_k)$ we maximize the following log odds of the posterior:

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$$

LDA is a special case of QDA. This is not surprising, since LDA is simply a restricted version of QDA with $\boldsymbol{\Sigma}_1 = \ldots = \boldsymbol{\sigma}_K = \boldsymbol{\Sigma}$.

Log odds of posterior probabilities in naive Bayes and LDA

In naive Bayes setting, $f_k(\mathbf{x}) = \prod_{p=1}^{P} f_{kp}(x_p)$, we maximize the following log odds:

$$\log\left(\frac{\mathbb{P}(Y=k|\mathbf{X}=\mathbf{x})}{\mathbb{P}(Y=K|\mathbf{X}=\mathbf{x})}\right) = \log\left(\frac{\mathbb{P}(Y=k)\mathbb{P}(\mathbf{X}=\mathbf{x}|Y=k)}{\mathbb{P}(Y=K)\mathbb{P}(\mathbf{X}=\mathbf{x}|Y=K)}\right) = \log\left(\frac{\pi_k \prod_{p=1}^{P} f_{kp}(x_p)}{\pi_K \prod_{p=1}^{P} f_{Kp}(x_p))}\right)$$

$$= \underbrace{\log\left(\frac{\pi_k}{\pi_K}\right)}_{\equiv a_k} + \sum_{p=1}^{P} \underbrace{\log\left(\frac{f_{kp}(x_p)}{f_{Kp}(x_p))}\right)}_{\equiv g_{kp}(x_p)} = a_k + \sum_{p=1}^{P} g_{kp}(x_p), \text{ generalized additive model,} \quad (10)$$

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$$= \underbrace{\log\left(\frac{\pi_k}{\pi_K}\right)}_{\equiv a_k} + \sum_{p=1}^{P} \underbrace{\log\left(\frac{f_{kp}(x_p)}{f_{Kp}(x_p))}\right)}_{\equiv g_{kp}(x_p)} = a_k + \sum_{p=1}^{P} g_{kp}(x_p), \text{ generalized additive model}, \tag{10}$$

where a_k, b_{kp}, c_{kpq} are functions of $\pi_k, \pi_K, \boldsymbol{\mu}_k, \boldsymbol{\mu}_K, \boldsymbol{\Sigma}_k, \boldsymbol{\Sigma}_K$.

Log odds of posterior probabilities in naive Bayes and LDA

In naive Bayes setting, $f_k(\mathbf{x}) = \prod_{p=1}^{P} f_{kp}(x_p)$, we maximize the following log odds:

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where a_k, b_{kp}, c_{kpq} are functions of $\pi_k, \pi_K, \boldsymbol{\mu}_k, \boldsymbol{\mu}_K, \boldsymbol{\Sigma}_k, \boldsymbol{\Sigma}_K$. Recall that for LDA:

$$\log\left(\frac{\mathbb{P}(Y=k|\mathbf{X}=\mathbf{x})}{\mathbb{P}(Y=K|\mathbf{X}=\mathbf{x})}\right) = a_k + \sum_{p=1}^{P} b_{kp} x_p, \text{ linear in } \mathbf{x}.$$

Log odds of posterior probabilities in naive Bayes and LDA

In naive Bayes setting, $f_k(\mathbf{x}) = \prod_{p=1}^{P} f_{kp}(x_p)$, we maximize the following log odds:

$$\log\left(\frac{\mathbb{P}(Y=k|\mathbf{X}=\mathbf{x})}{\mathbb{P}(Y=K|\mathbf{X}=\mathbf{x})}\right) = \log\left(\frac{\mathbb{P}(Y=k)\mathbb{P}(\mathbf{X}=\mathbf{x}|Y=k)}{\mathbb{P}(Y=K)\mathbb{P}(\mathbf{X}=\mathbf{x}|Y=K)}\right) = \log\left(\frac{\pi_k \prod_{p=1}^{P} f_{kp}(x_p)}{\pi_K \prod_{p=1}^{P} f_{Kp}(x_p))}\right)$$

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$$\log\left(\frac{\mathbb{P}(Y=k|\mathbf{X}=\mathbf{x})}{\mathbb{P}(Y=K|\mathbf{X}=\mathbf{x})}\right) = a_k + \sum_{p=1}^{P} b_{kp}x_p, \text{ linear in } \mathbf{x}.$$

Any classifier with a linear decision boundary is a special case of naive Bayes with $g_{kp}(x_p) = b_{kp}x_p$.

Log odds of posterior probabilities in naive Bayes and LDA

In naive Bayes setting, $f_k(\mathbf{x}) = \prod_{p=1}^{P} f_{kp}(x_p)$, we maximize the following log odds:

$$\log\left(\frac{\mathbb{P}(Y=k|\mathbf{X}=\mathbf{x})}{\mathbb{P}(Y=K|\mathbf{X}=\mathbf{x})}\right) = \log\left(\frac{\mathbb{P}(Y=k)\mathbb{P}(\mathbf{X}=\mathbf{x}|Y=k)}{\mathbb{P}(Y=K)\mathbb{P}(\mathbf{X}=\mathbf{x}|Y=K)}\right) = \log\left(\frac{\pi_k \prod_{p=1}^{P} f_{kp}(x_p)}{\pi_K \prod_{p=1}^{P} f_{Kp}(x_p))}\right)$$

$$= \underbrace{\log\left(\frac{\pi_k}{\pi_K}\right)}_{\equiv a_k} + \sum_{p=1}^{P} \underbrace{\log\left(\frac{f_{kp}(x_p)}{f_{Kp}(x_p))}\right)}_{\equiv g_{kp}(x_p)} = a_k + \sum_{p=1}^{P} g_{kp}(x_p), \text{ generalized additive model,} \tag{10}$$

where a_k, b_{kp}, c_{kpq} are functions of $\pi_k, \pi_K, \boldsymbol{\mu}_k, \boldsymbol{\mu}_K, \boldsymbol{\Sigma}_k, \boldsymbol{\Sigma}_K$. Recall that for LDA:

$$\log\left(\frac{\mathbb{P}(Y=k|\mathbf{X}=\mathbf{x})}{\mathbb{P}(Y=K|\mathbf{X}=\mathbf{x})}\right) = a_k + \sum_{p=1}^{P} b_{kp}x_p, \text{ linear in } \mathbf{x}.$$

Any classifier with a linear decision boundary is a special case of naive Bayes with $g_{kp}(x_p) = b_{kp}x_p$. This means that this means that LDA is a special case of naive Bayes!

Log odds of posterior probabilities in naive Bayes and LDA

In naive Bayes setting, $f_k(\mathbf{x}) = \prod_{p=1}^{P} f_{kp}(x_p)$, we maximize the following log odds:

$$\log\left(\frac{\mathbb{P}(Y=k|\mathbf{X}=\mathbf{x})}{\mathbb{P}(Y=K|\mathbf{X}=\mathbf{x})}\right) = \log\left(\frac{\mathbb{P}(Y=k)\mathbb{P}(\mathbf{X}=\mathbf{x}|Y=k)}{\mathbb{P}(Y=K)\mathbb{P}(\mathbf{X}=\mathbf{x}|Y=K)}\right) = \log\left(\frac{\pi_k \prod_{p=1}^{P} f_{kp}(x_p)}{\pi_K \prod_{p=1}^{P} f_{Kp}(x_p))}\right)$$

$$= \underbrace{\log\left(\frac{\pi_k}{\pi_K}\right)}_{\equiv a_k} + \sum_{p=1}^{P} \underbrace{\log\left(\frac{f_{kp}(x_p)}{f_{Kp}(x_p))}\right)}_{\equiv g_{kp}(x_p)} = a_k + \sum_{p=1}^{P} g_{kp}(x_p), \text{ generalized additive model,} \quad (10)$$

where a_k, b_{kp}, c_{kpq} are functions of $\pi_k, \pi_K, \boldsymbol{\mu}_k, \boldsymbol{\mu}_K, \boldsymbol{\Sigma}_k, \boldsymbol{\Sigma}_K$. Recall that for LDA:

$$\log\left(\frac{\mathbb{P}(Y=k|\mathbf{X}=\mathbf{x})}{\mathbb{P}(Y=K|\mathbf{X}=\mathbf{x})}\right) = a_k + \sum_{p=1}^{P} b_{kp}x_p, \text{ linear in } \mathbf{x}.$$

Any classifier with a linear decision boundary is a special case of naive Bayes with $g_{kp}(x_p) = b_{kp}x_p$. This means that this means that LDA is a special case of naive Bayes!

This is a little bit surprising!

Log odds of posterior probabilities in naive Bayes and LDA

In naive Bayes setting, $f_k(\mathbf{x}) = \prod_{p=1}^{P} f_{kp}(x_p)$, we maximize the following log odds:

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$$= \underbrace{\log\left(\frac{\pi_k}{\pi_K}\right)}_{\equiv a_k} + \sum_{p=1}^{P} \underbrace{\log\left(\frac{f_{kp}(x_p)}{f_{Kp}(x_p))}\right)}_{\equiv g_{kp}(x_p)} = a_k + \sum_{p=1}^{P} g_{kp}(x_p), \text{ generalized additive model,} \tag{10}$$

where a_k, b_{kp}, c_{kpq} are functions of $\pi_k, \pi_K, \boldsymbol{\mu}_k, \boldsymbol{\mu}_K, \boldsymbol{\Sigma}_k, \boldsymbol{\Sigma}_K$. Recall that for LDA:

$$\log\left(\frac{\mathbb{P}(Y=k|\mathbf{X}=\mathbf{x})}{\mathbb{P}(Y=K|\mathbf{X}=\mathbf{x})}\right) = a_k + \sum_{p=1}^{P} b_{kp} x_p, \text{ linear in } \mathbf{x}.$$

Any classifier with a linear decision boundary is a special case of naive Bayes with $g_{kp}(x_p) = b_{kp}x_p$. This means that this means that LDA is a special case of naive Bayes!

This is a little bit surprising!

Each method makes very different assumptions:

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Each method makes very different assumptions: LDA assumes that the features are normally distributed with a common within-class covariance matrix, and naive Bayes instead assumes independence of the features.

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If we model $f_{kp}(x_p) = \mathcal{N}(\mu_{kp}, \sigma_p^2)$, then we end up with $g_{kp}(x_p) = b_{kp}x_p$, where $b_{kp} \equiv (\mu_{kp} - \mu_{Kp})/\sigma_p^2$. In this case, naive Bayes, is actually a special case of LDA with $\boldsymbol{\Sigma}$ restricted to be a diagonal matrix with pth diagonal element equal to σ_p^2.

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Therefore, QDA has the potential to be more accurate in settings where interactions among the predictors are important in discriminating between classes.

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