Computational Statistics

Beyond Linear

In practice, linear methods are inevitably approximations. Many non-linear methods can be derived as generalizations of linear methods.

Quadratic discriminant analysis (QDA) models the conditional distribution of x given y=k as a multivariate normal distribution, but unlike LDA, does not assume a common covariance matrix for each class.

$$h_k(x \mid \mu_k, \Sigma_k) = |2\pi\Sigma_k|^{-1/2} \exp\left(-\frac{1}{2}(x - \mu_k)\Sigma_k^{-1}(x - \mu_k)^T\right).$$

parameter estimation

To estimate the parameters of the QDA model from training data,

1. marginal probabilities

$$\hat{q}_k = n_k/n$$

2. conditional means

$$\hat{\mu}_k = \sum_{y_i = k} x_i / n_k$$

3. covariance matrices

$$\hat{\Sigma}_k = \sum_{\{i:y_i=k\}} (x_i - \hat{\mu}_k)(x_i - \hat{\mu}_k)/(n_k - 1).$$

where n is the number of observations in the training data, and n_k is the number of observations in the training data with $y_i = k, k = 1, ..., K$.

The discriminant for QDA is

$$\delta_k(x) = \frac{h_k(x)\hat{q}_k}{h(x)}$$

$$= \frac{\hat{q}_k}{h(x)\sqrt{2\pi|\hat{\Sigma}_k|}} \exp\left(-\frac{1}{2}(x-\hat{\mu}_k)\hat{\Sigma}_k^{-1}(x-\hat{\mu}_k)'\right).$$

Omitting the multiplicative terms that do not depend on k, we get the simplified version,

$$\delta_k(x) = \frac{\hat{q}_k}{\sqrt{|\hat{\Sigma}_k|}} \exp\left(-\frac{1}{2}(x - \hat{\mu}_k)\hat{\Sigma}_k^{-1}(x - \hat{\mu}_k)'\right).$$

Taking a log transformation, the discriminant for QDA is

$$\log \delta_{k}(x) = \log(\hat{q}_{k}) - \frac{1}{2}\log(|\hat{\Sigma}_{k}|) - \frac{1}{2}(x - \hat{\mu}_{k})\hat{\Sigma}_{k}^{-1}(x - \hat{\mu}_{k})'$$

$$= \log(\hat{q}_{k}) - \frac{1}{2}\log(|\hat{\Sigma}_{k}|) - \frac{1}{2}x\hat{\Sigma}_{k}^{-1}x' + x\hat{\Sigma}_{k}^{-1}\hat{\mu}_{k} - \frac{1}{2}\hat{\mu}_{k}\hat{\Sigma}_{k}^{-1}\hat{\mu}_{k}'.$$

which is a quadratic function of x (unlike LDA, which was linear in x).