Statistical learning notes

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Contents

1 Introducton

Before going into the data analysis, try to visualize it to have a first impression.
Difference between machine learning and statistical learning:

- Machine learning has a greater emphasis on *large scale* applications and *prediction accuracy*.
- Statistical learning emphasizes *models* and their interpretability, and *precision* and *uncertainty*.

The supervised learning problem:

- Outcome meansure Y also called dependent variable, reponse, target.
- Vector of p predictor measurements X also called inputs, regressors, covariates, features, independent variables.
- In the *regression problem*, Y is quantitative (e.g. price, blood pressure).
- In the *classification problem*, Y takes values in a finite, unordered set.
- We have training data. These are observations of these measurements.

On the basis of the training data we would like to

- Accurately predict unseen test cases.
- Understand which inputs affect the outcome and how
- Assess the quality of our predictions and inferences.

To apply supervised learning, one has to understand the simple methods first, in order to grasp the more sophsiticated ones. It is important to accurately assess the performance of a method, to know how well or how badly it is working.

In unsupervised learning,

- No output/dependent variable (response), just a set of predictors (features) measured on a set of samples.
- objective is more fuzzy — find groups of samples that behave similarly, find features that behave similarly, find linear combinations of features with the most variation.
- difficult to evaluate the method.
- can be used as a pre-processing step for supervised learning.

We denote the input vector as

$$X = \begin{pmatrix} X_1 \\ X_2 \\ X_3 \end{pmatrix},$$

where X refers to the variable and x denotes as the instance, and we usually take column vectors.
The ideal $f(x) = E(Y|X = x)$ is called the regression function.

- The regression function $\hat{f}(x)$ is the ideal or optimal predictor of Y with regard to mean-squared predictor of Y with regard to mean-squared prediction error: $f(x) = E(Y|X = x)$ is the function taht minimize $E[(Y - g(X))^2|X = x]$ over all functions g at all points $X = x$.
- We also have $\varepsilon = Y - f(x)$ as the irreducible error.
- For any estimate $\hat{f}(x)$ of $f(x)$, we have
$$E[(Y - \hat{f}(X))^2|X = x] = [f(x) - \hat{f}(x)]^2 + \mathrm{Var}(\varepsilon).$$
- We relax the definition and let
$$\hat{f}(x) = \mathrm{Ave}(Y|X \in \mathrm{N}(x)),$$
where $\mathrm{N}(x)$ is some *neighborhood* of x.
- Nearest neighbor average can be pretty good for small number of components p, i.e. $p \leq 4$ and large N.
- Nearest neighbors tend to far away in high dimensions. (Curse of dimensionality). Note the curve about the curse of dimensionality. NN is to have the average estimate whose variance is 10% lower than the original data. A 10% neighborhood in high dimensions need no longer be local, so we cannot estimate $E(Y|X = x)$ by local averaging.

Some trade-offs:

- Prediction accuracy versus interpretability
- Good fit versus over-fit or under-fit
- Parsimony versus black-box

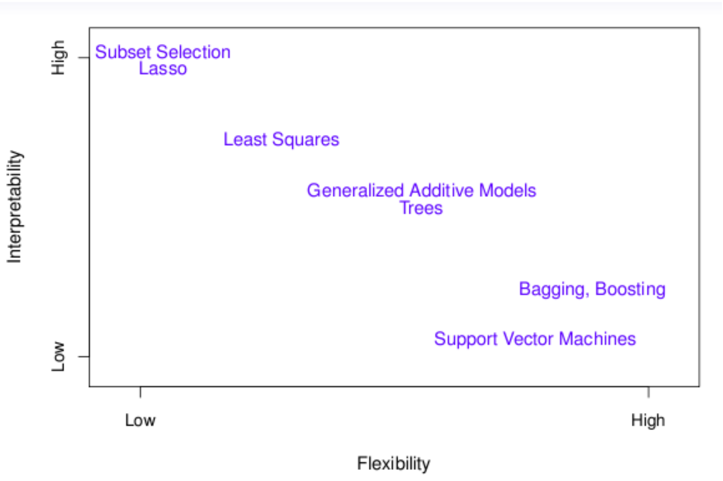


Figure 1: Interpretability vs flexibility.

We also have the Bias-Variance Trade-Off: The expected test MSE is

$$E(y_0 - \hat{f}(x_0))^2 = \mathrm{Var}(\hat{f}(x_0)) + [\mathrm{Bias}(\hat{f}(x_0))]^2 + \mathrm{Var}(\varepsilon).$$

- The variance of a statistical learning method refers to the amount by which $\hat{f}$ would change if we estimated it using a different training dataset. In general, more flexible methods have higher variance.

- The Bias refers to the error that is introduced by approximating a real-life problem, which may be extremely complicated, by a much simpler model.
- As a general rule, as we use more flexible methods, the variance will increase and the bias will decrease. The relative rate of change of these two quantities determines whether the test MSE increases or decreases.

For classification, the Bayes optimal classifier at x is

$$C(x) = j \text{ if } p_j(x) = \max\{p_1(x), p_2(x), \ldots, p_K(x)\},$$

where the conditional class probabilities at x is

$$p_k(x) = \Pr(Y = k|X = x), k = 1, 2, \ldots, K.$$

- The performance of $\hat{C}(x)$ using the misclassification error rate is:

$$\mathrm{Err}_{\mathbf{Te}} = \underset{i\in\mathbf{Te}}{\mathrm{Ave}}\, I[y_i \neq \hat{C}(x_i)].$$

For K-nearest neighbor, increasing K will reduce the training error continuously, but test error first drops and then rises.

2 Linear Regression

Linear regression is a simple approach to supervised learning. It assumes that the dependence of Y on $X_1, X_2, \ldots, Xp$ is linear.
We assume a model

$$Y = \beta_0 + \beta_1 X + \varepsilon,$$

where β_0 and β_1 are two unknown constants that represent the intercept and slope, also known as *coefficients* or *parameters*, and ε is the error term. Given some estiamtes $\hat{\beta}_0$ and $\hat{\beta}_1$ for the model coefficients, we have the prediction

$$\hat{y} = \hat{\beta}_0 + \hat{\beta}_1 x,$$

where $\hat{y}$ indicates a prediction of Y on the basis of $X = x$.
Estimation of the parameters by least squares

- We define $e_i = y_i - \hat{y}_i$ as the ith *residual*, Then the *residual sum of squares* (RSS) is defined as

$$\begin{aligned}(RSS) &= e_1^2 + e_2^2 + \cdots + e_n^2,\\ &= (y_1 - \hat{\beta}_0 - \hat{\beta}_1 x_1)^2 + (y_2 - \hat{\beta}_0 - \hat{\beta}_1 x_2)^2 + \cdots + (y_n - \hat{\beta}_0 - \hat{\beta}_1 x_n)^2.\end{aligned}$$

- The least squares approach chooses $\hat{\beta}_0$ and $\hat{\beta}_1$ to minimize the RSS. The minimizing values are

$$\begin{aligned}\hat{\beta}_0 &= \bar{y} - \hat{\beta}_1 \bar{x},\\ \hat{\beta}_1 &= \frac{\sum_{i=1}^n (x_i - \bar{x})(y_i - \bar{y})}{\sum_{i=1}^n (x_i - \bar{x})^2},\end{aligned}$$

where $\bar{y} = \frac{1}{n}\sum_{i=1}^n y_i$ and $\bar{x} = \frac{1}{n}\sum_{i=1}^n x_i$ are the sample means.

We could also write the estimation of β_1 in matrix form as follows.

$$\hat{\beta}_1 = \frac{C_{xy}}{C_{xx}} = \rho \cdot \frac{\sqrt{C_{yy}}}{\sqrt{C_{xx}}},$$

where we denote the corrlation matrix as $\rho = \frac{C_{xy}}{\sqrt{C_{xx}} \cdot \sqrt{C_{yy}}}$. The cross-covariance matrix $C_{xy} = \mathbf{X}(\mathbf{I} - \frac{1}{N}\mathbf{e}\mathbf{e}^\top)\mathbf{Y}^\top$.

2.1 Assessing the accuracy of the coefficient estimates

Suppose we have random sample $x_1, x_2, \dots, x_n$. The standard error of the mean (SEM) is the standard deviation of the sample-mean's estimate of a population mean.

$$\text{SE}_{\bar{x}} = \frac{s}{\sqrt{n}}$$

where s is the sample standard deviation and n is the number of observations of the sample.
This estimate can be cmopared with the formula for the true standard deviation of the sample mean as T/n as $T = (x_1, x_2, \dots, x_n)$:

$$\text{SD}_{\bar{x}} = \frac{\sigma}{\sqrt{n}}.$$

The standard errors associated with $\hat{\beta}_0$ and $\hat{\beta}_1$ are

$$\text{SE}(\hat{\beta}_1)^2 = \frac{\sigma^2}{\sum_{i=1}^{n}(x_i - \bar{x})^2}$$

$$\text{SE}(\hat{\beta}_0)^2 = \sigma^2[\frac{1}{n} + \frac{\bar{x}^2}{\sum_{i=1}^{n}(x_i - \bar{x})^2}]$$

Confidence interval:
A 95% confidence interval is defined as a range of values such that 95% probability, the range will contain the true unknown value of the parameter, i.e. $\hat{\beta}_1 \pm 2 \cdot \text{SE}(\hat{\beta}_1)$. This is a frequentist idea.

Standard errors can also be used to perform hypothesis tests on the coefficients.

- To test the null hypothesis, we compute a *t-statistic*, given by

  $$t = \frac{\hat{\beta}_1 - 0}{\text{SE}(\hat{\beta}_1)},$$

  It measures the number of standard deviations that $\hat{\beta}_1$ is away from 0.

- This will have a t-distribution with $n-2$ degrees of freedom, assuming $\beta_1 = 0$.

- Using statistical tools, we can compute the probability of observing any value equal to $|t|$ or larger. We call this probability the *p-value*.

- We interpret the p-value as follows: with a small p-value we can infer there is an association between the predictor and the response.

Degree of freedom:

- In statistics, the number of degrees of freedom is the number of values in the final calculation of a statistic that are free to vary. It is the number of independent observations in a sample of data that are available to estimate a parameter of the population from which that sample is drawn.

- In general, the degrees of freedom of an estimate of a parameter are equal to the number of independent scores that go into the estimate minus the number of parameters used as intermediate steps in the estimation of the parameter itself, e.g. the sample variance has N-1 degrees of freedom, since it is computed from N random scores minus the only 1 parameter estimated as intermediate step, which is the sample mean.

Assessing the overal accuracy of the model

- We comptue the *Residual Standard Error*

$$\mathrm{RSE} = \sqrt{\frac{1}{n-2}\mathrm{RSS}} = \sqrt{\frac{1}{n-2}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2},$$

  where the residual sum-of-squares is $\mathrm{RSS} = \sum_{i=1}^{n}(y_i - \hat{y}_i)^2$.

- *R-squared* or fraction of variance explained is

$$R^2 = \frac{\mathrm{TSS} - \mathrm{RSS}}{\mathrm{TSS}} = 1 - \frac{\mathrm{RSS}}{\mathrm{TSS}}.$$

  where $\mathrm{TSS} = \sum_{i=1}^{n}(y_i - \bar{y}_i)^2$ is the total sum of squares (TSS).
  R^2 is easier to interprete than RSE as it is between 0 and 1, but sometimes hard to determine what is a good R^2 value.

- The R^2 statistic is the correlation between the two variables and measures how closely the input variable and the output variable are related. The p value and t statistic merely measure how strong is the evidence that there is a nonzero association. Even a weak effect can be extremely significant given enough data.

Multiple Linear Regression:
It refers to regression models wth more than one predictor.

- Model: $Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \beta_3 X_3$
- we interpret β_j as the *average* effect on Y of a one unit increase in X_j, holding all other predictors fixed.

Interpreting regression coefficients

- The ideal scenario is when the predictors are uncorrelated:
  - Each coefficient can be estimated and tested separately
  - We can have the response depend on one predictors, with others fixed.
- The variance of all coefficients tends to increase, sometimes dramatically
- Interpretations become hazadous
- Claims of causality should be avoided for observational data.

Estimation and Prediction for Multiple Regression

- Given estimates $\hat{\beta}_0, \hat{\beta}_1, \ldots, \hat{\beta}_p$, we can make predictions using the formula

$$\hat{y} = \hat{\beta}_0 + \hat{\beta}_1 x_1 + \hat{\beta}_2 x_2 + \cdots + \hat{\beta}_p x_p$$

- The sum of squared residuals is

$$\begin{aligned} \mathrm{RSS} &= \sum_{i=1}^{n}(y_i - \hat{y}_i)^2 \qquad (1)\\ &= \sum_{i=1}^{n}(y_i - \hat{\beta}_0 - \hat{\beta}_1 x_{i1} - \hat{\beta}_2 x_{i2} - \cdots - \hat{\beta}_p x_{ip})^2. \qquad (2) \end{aligned}$$

  The values $\hat{\beta}_0, \hat{\beta}_1, \ldots, \hat{\beta}_p$ minimize RSS are the multiple least squares regression coefficient estimates.

We define F-statistics

$$F = \frac{(\mathrm{TSS} - \mathrm{RSS}/p)}{\mathrm{RSS}/(n-p-1)} \sim F_{p,n-p-1}.$$

- If F-statistics is far larger than 1, it shows it is against the null hypothesis H_0.
- If F-statistic is significant, then we have extremely strong evidence that at least one of the predictors is associated with response.
- If n is large, an F-statistic that is just a little larger than 1 might still provide evidence against H_0, and vice versa.
- When H_0 is true and the errors ε_i have a normal distribution, the F-statistic follows an F-distribution.
- We can compute p-value from the F-statistic. And we can determine whether or not to reject H_0 based on the p-value.
- There is a high chance to incorrectly conclude there is an association between the variable and the responce based on the individual t-statistics and associated p-values. The F-statistic does not suffer from this problem because it adjusts for the number of predictors.
- If $p > n$ then there are more coefficients β_j to estimate than observations from which to estimate them. We cannot fit the multiple linear regression model using least squares, so F-statistics cannot be used.

Deciding on the important variables

- Forward selection: begin with the null model and add p simple linear regressions that reults in the lowest RSS, until a stopping criterion is met.
- Backward selection: start with all variables in the model. Remove the one with the largest p-value iteratively, until a stopping criterion is met.

Qualitative Predictors

- They are discrete set of values.
- Also called categorical predictors or factor variables.

Removing the additive assumption: *interactions* and *nonlinearity*.

- One input variable can influence another variable.
- We can use the multiplication of the interacted variables to check the p-value of coefficent. It p-value is low, it indicates a strong interaction.

Polynomial regression is the linear regression with non-linear regression functions.

The hierarchy principle: If we include an interaction in a model, we should also include the main effects, even if the p-values assocated with their coefficients are not significant.
We can also have linear coefficients but non-linear functions of variable.

Outliers

Non-constant variance of error terms

High leverage points

Collinearity

Statistical variability

Scatter plot and box plot are two most common data visualization methods. For box plot

- The bottom and top of the box are always the first and third quartiles, and the band inside the box is always the second quartile (the median).
- The very bottom and top line are the hinges, which are the ranges.

3 Classification

We can use Linear Regression for binary classification problems, which is equivalent to *linear discriminant analysis*. $E(Y|X=x) = \Pr(Y=1|X=x)$. But for multiclass problems, we cannot use linear regression.

3.1 Logistic Regression:

We have $p(X) = \Pr(Y=1|X)$ and it has the form

$$p(X) = \frac{e^{\beta_0+\beta_1 X}}{1+e^{\beta_0+\beta_1 X}}$$

$p(X) \in [0,1]$.
We also have the *log odds* or *logit transformation* of $p(X)$ as

$$\log(\frac{p(X)}{1-p(X)}) = \beta_0 + \beta_1 X.$$

We use maximium likelihood to estimate the parameters.

$$\ell(\beta_0, \beta) = \prod_{i:y_i=1} p(x_i) \prod_{i:y_i=0} (1-p(x_i)).$$

The likelihood gives the probabilitiy of the observed zeros and oens in the data. We pick β_0 and β_1 to maximize the likelihood of the observed data.
Logistic regression with several variables

$$\log(\frac{p(X)}{1-p(X)}) = \beta_0 + \beta_1 X_1 + \cdots + \beta_p X_p$$

$$p(X) = \frac{e^{\beta_0+\beta_1 X_1+\cdots+\beta_p X_p}}{1+e^{\beta_0+\beta_1 X_1+\cdots+\beta_p X_p}}.$$

Confounding
Scatter plot: a type of mathematical diagram using Cartesian coordinates to display values for typically two variables for a set of data. If the points are color-coded you can increase the number of displayed variables to three.

Tilde in R:
The thing on the right of $\leftarrow$ is a formula object. It is often used to denote a statistical model, where the thing on the left of the $\sim$ is the response and the things on the right of the $\sim$ are the explanatory variables. So in English you'd say something like "Species depends on Sepal Length, Sepal Width, Petal Length and Petal Width".
Data Frame: The concept of a data frame comes from the world of statistical software used in empirical research; it generally refers to "tabular" data: a data structure representing cases (rows), each of which consists of a number of observations or measurements (columns). Alternatively, each row may be treated

as a single observation of multiple "variables". In any case, each row and each column has the same data type, but the row ("record") datatype may be heterogenous (a tuple of different types), while the column datatype must be homogenous. Data frames usually contain some metadata in addition to data; for example, column and row names.

Case-control sampling and logistic regression

- With case-control samples, we can estimate the regression parameters β_j accurately if our model is correct, the constant term β_0 is incorrect.
- We can correct the estimated intercept by a simple transformation

  $$\hat{\beta}_0^* = \hat{\beta}_0 + \log \frac{\pi}{1-\pi} - \log \frac{\tilde{\pi}}{1-\tilde{\pi}},$$

  where π is the true probability and $\tilde{\pi}$ is the case probability.
- Often cases are rare and we take them all; up to five times that number of controls is sufficient.
- Case/Control sampling is most effective when the prior probabilities of the classes are very unequal. We expect this to be the case for the cancer and spam problems, but not the gender problem.

Logistic regression with more than two classes

- One version used in R package *glmnet* (Softmax function). It has the symmetric from

  $$\Pr(Y=k|X) = \frac{e^{\beta_{0k}+\beta_{1k}X_1+\cdots+\beta_{pk}X_p}}{\sum_{\ell=1}^{K} e^{\beta_{0\ell}+\beta_{1\ell}X_1+\cdots+\beta_{p\ell}X_p}},$$

  where K is the number of classes, and $K > 2$. Each class has a linear function, and we weight against each other using an exponential function.
- It is also referred to as multinomial regression.

3.2 Discriminant Analysis

- It models the distribution of X in each of the classes separately, and then use *Bayes theorem* to flip things around and obtain $\Pr(Y|X)$.
- When we use normal distributions for each class, it leads to linear or quadratic discriminant analysis.
- It is quite generic, and applies to other distributions as well.

Bayes theorem for classification From the Bayes theorem,

$$\Pr(Y=k|X=x) = \frac{\Pr(X=x|Y=k)\cdot\Pr(Y=k)}{\Pr(X=x)},$$

Or

$$P(Y \mid X) = \frac{P(X \mid Y)}{\sum_i P(X \mid Y_i)P(Y_i)} \cdot P(Y)$$

we can write the discriminant analysis as

$$\Pr(Y=k|X=x) = \frac{\pi_k f_k(x)}{\sum_{l=1}^{K} \pi_l f_l(x)},$$

where $f_k(x) = \Pr(X=x|Y=k)$ is the density for X in class k, and we use normal densities separately for each class. $\pi_k = \Pr(Y=k)$ is the marginal or *prior* probability for class k.

Comparison between Logistic Regression and Discriminant Analysis

- When the classes are well-separated, the parameter estimates for the logistic regression model are unstable. Linear Disciminant Analysis (LDA) does not suffer from this problem.
- If n is small and the distribution of the predictors X is approximately normal in each of the classes, LDA is more stable.
- LDA is popular when we have more than two classes, because is also provides low-dimensional views of the data.

Linear Discriminant Analysis when $p = 1$

$$f_k(x) \sim \mathcal{N}(\mu_k, \sigma_k^2),$$

where μ_k and σ_k^2 are the mean and variance of class k respectively, and we assume all $\sigma_k = \sigma$ are the same.
We can plug in the former equation into the bayes formula. and perform some cancellation and simplification. To classify $X = x$, we need to find the largest $p_k(x)$. Taking logs, and discarding terms that do not depend on k, we see that it is equivalent to assigning x to the class with the largest *discriminant score*:

$$\delta_k(x) = x \cdot \frac{\mu_k}{\sigma^2} - \frac{\mu_k^2}{\sigma^2} + \log(\pi_k).$$

$\delta_k(x)$ is a **linear** function of x. Parameter estimation

$$\hat{\pi}_k = \frac{n_k}{n} \tag{3}$$

$$\hat{\mu}_k = \frac{1}{n_k} \sum_{i:y_i=k} x_k \tag{4}$$

$$\hat{\sigma}^2 = \frac{1}{n-K} \sum_{k=1}^{K} \sum_{i:y_i=k} (x_i - \hat{\mu}_k)^2 \tag{5}$$

$$= \sum_{k=1}^{K} \frac{n_k - 1}{n-K} \cdot \hat{\sigma}_k^2. \tag{6}$$

where $\hat{\sigma}_k^2 = \frac{1}{n_k-1} \sum_{i:y_i=k} (x_i - \hat{\mu}_k)^2$ is the usual formula for the estimated variance in the kth class.
Linear Discriminant Analysis when $p > 1$
Density:

$$f(x) = \frac{1}{(2\pi)^{p/2} |\Sigma|^{1/2}} e^{-\frac{1}{2}(x-\mu)^\top \Sigma^{-1} (x-\mu)}.$$

Discriminant function:

$$\delta_k(x) = x^\top \Sigma^{-1} \mu_k - \frac{1}{2} \mu_k^T \Sigma^{-1} \mu_k + \log \pi_k.$$

but it remains linear.
Fisher's Disciminant Plot:
When there are K classes, linear discriminant analysis can be viewed in a $K - 1$ dimensional plot. It classifies to the closest centroid, and they span a $K - 1$ dimensional plane.

Probabilisitic interpretation
Once we have estimates $\hat{\delta_k}(x)$, we can turn these functions into estimates for class probabilities:

$$\hat{\Pr}(Y = k | X = x) = \frac{e^{\hat{\delta}_k(x)}}{\sum_{l=1}^{K} e^{\hat{\delta}_l(x)}}.$$

The ROC curve shows true positive rate and false positive rate simultaneously. The curve traces out when changing the threshold. We also use the AUC or area under the curve to compare the performance between classifiers with different thresholds. Higher AUC is good.

Other forms of Discriminant Analysis

$$\Pr(Y = k|X = x) = \frac{\pi_k f_k(x)}{\sum_{l=1}^{K} \pi_l f_l(x)}$$

When $f_k(x)$ are Gaussian densities, with the same covariance matrix Σ in each class, it leads to LDA. By altering the forms for $f_k(x)$, we get different classifiers as

- With Gaussians but different Σ_k in each class, we get quadratic discriminant analysis.
- With $f_k(x) = \prod_{j=1}^{p} f_{jk}(x_j)$ (conditional independence model) in each class we get naive Bayes. For Gaussian this means the Σ_k are diagonal.
- Many other forms, by proposing specific density models for $f_k(x)$, including nonparametric approaches.

Quadratic Discriminant Analysis

$$\delta_k(x) = -\frac{1}{2}(x-\mu_k)^\top \Sigma_k^{-1}(x-\mu_k) + \log \pi_k - \frac{1}{2}\log|\Sigma_k|$$

The quandratic terms matter as Σ_k are different.

Naive Bayes

Assume features are independent in each class. NB is Useful when p is large, and multiviariate methods like QDA and even LDA break down due to large covariance matrices.

- Gaussian naive Baye assumes each Σ_k is diagonal:

$$\begin{aligned} \delta_k(x) &\sim \log\left[\pi_k \prod_{j=1}^{p} f_{ij}(x_j)\right] & (7) \\ &= -\frac{1}{2}\sum_{j=1}^{p}\left[\frac{(x_j-\mu_{kj})^2}{\sigma_{kj}^2} + \log \sigma_{kj}^2\right] + \log \pi_k. & (8) \end{aligned}$$

- can use for mixed feature vectors (qualitative and quantitative). If X_j is qualitative, replace $f_{kj}(X_j)$ with probability mass function (histogram) over discrete categories.

Compare Logistic Regression and LDA

For a two-class problem, one can show for LDA

$$\log\left(\frac{p_1(x)}{1-p_1(x)}\right) = \log\left(\frac{p_1(x)}{p_2(x)}\right) = c_0 + c_1 x_1 + \cdots + c_p x_p.$$

It has the same form as logistic regression. The difference is in how the parameters are estimated.

- Logistic regression uses the conditional likelihood based on $\Pr(Y|X)$, known as discriminative learning.
- LDA uses the full likelihood based on $\Pr(X,Y)$, known as generative learning.
- Despite these differences, in practice the results are often very similar.

4 Resampling

Validation method: We split the original training set into a train and validation set. Then, we fit models of various set sizes and of various model sizes. Our job is to find $\hat{k}$, and return the model $\mathcal{M}_{\hat{k}}$.

- two major methods: cross validation and the bootstrap
- Resampling refits a model of interest to samples formed from the training set, in order to obtain addtional information about the fitted model.
- They provide estimates of test set prediction error, and the standard deviation and bias of our parameter estimates.

Drawbacks of validation set approach

- the validation estimate of the test error can be highly variable, depending on precisely which observations are included in the training set and which observations are included in the validation set
- Only a subset of the observation are used for training
- The validation set error may tend to overestimate the test error for the model fit on the entire dataset.

K-fold cross validation

- random divides the data into K equal-size parts. We leave out. We leave out part k, fit the model to the other $K-1$ parts (combined), and then obtain predictions for the left-out kth part.
- Let the K parts be $C_1, C_2, \dots C_K$ where C_k denotes the indices of the observations in part k. There are n_k observations in part k: if N is a multiple of K, then $n_k = n/K$.
- Computer

  $$CV_{(K)} = \sum_{k=1}^{K} \frac{n_k}{n} \text{MSE}_k,$$

  where $\text{MSE}_k \sum_{i \in C_k} (y_i - \hat{y}_i)^2 / n_k$ and $\hat{y}_i$ is the fit for observation i, obtained from the data with part k removed.
- Setting $K = n$ yield n-fold or leave-one out cross validation.

Leave-one-out cross validation

- With least squares linear or polynomial regression, an amazing shortcut maeks the cost of leave-one out cross validation the same as that of a single model fit.

  $$\text{CV}_{(n)} = \frac{1}{n} \sum_{i=1}^{n} \left(\frac{y_i - \hat{y}_i}{1 - h_i} \right)^2.$$

  where $\hat{y}_i$ is the $i$the fitted value from the original least squares fit, and h_i is the leverage. It is like the ordinary MSR, except the $i$the residual is divided by $1 - h_i$.
- It does not shake up the data enough. The estimates from each fold are highly correlated and hence their average can have high variance.
- $K = 5, 10$ is a better choice.

Problems with Cross validation

- Since each training set is only $(K-1)/K$ as big as the original training set, the estimates of prediction error will typically be biased upward.
- The biase is minimized when $K=n$ (leave one out), the estimae has high variance.
- $K=5\text{or}10$ provides a better compromise.

Cross Validation for Classification

- Compute

$$CV_K = \sum_{k=1}^{K} \frac{n_k}{n} \mathrm{Err}_k$$

  where $\mathrm{Err}_k = \sum_{i \in C_k} I(y_i \neq \hat{y}_i)/n_k$.

- The estimated standard deviation of CV_k is

$$\hat{\mathrm{SE}}(CV_k) = \sqrt{\sum_{k=1}^{K} \mathrm{Err}_k - \bar{\mathrm{Err}}_k^{\,2}/(K-1)}.$$

Cross validation: right and wrong

- If we pre-select the predictors correlated to the class labels, we should not ignore this fact when applying cross validation. The procedure has already seen the labels of the training data and made use of them. It is a form of training and should be included in the validation process.
- The right way is to apply screening and validation at each round of cross validation.

The bootstrap

- For real data, we cannot generate new samples from the original population.
- Bootstrap allows to use computer to mimic the processing of obtaining new data sets, so that we can estimate the variability of our estimate without generating additonal samples.
- Rather than repeatedly obtaining independent datasets from the population, we obtain distinct datasets by repeatedly sampling obserations from the original dataset with *replacement*.
- The procedure is repeated B times for some large value of B, in order to produce B different bootstrap datasets, $Z^{*1}, Z^{*2}, \ldots Z^{*B}$ and B corresponding α estimates, $\hat{\alpha}^{*1}, \hat{\alpha}^{*2} \ldots \hat{\alpha}^{*B}$.
- We estimate the standard error of these bootstrap estimates using the formula

$$\mathrm{SE}_B(\hat{\alpha}) = \sqrt{\frac{1}{B-1} \sum_{r=1}^{B} (\hat{\alpha}^{*r} - \bar{\hat{\alpha}}^{*})^2}$$

- In time series data, where data is not iid., we cannot bootstrap the data with replacement, but we can apply block boostrap.
- Primarily used to obtain standard erros of an estimate
- also provides approximate confidence intervals for a population parameter, which represents an approximate 90% confidence intervial for the true α.

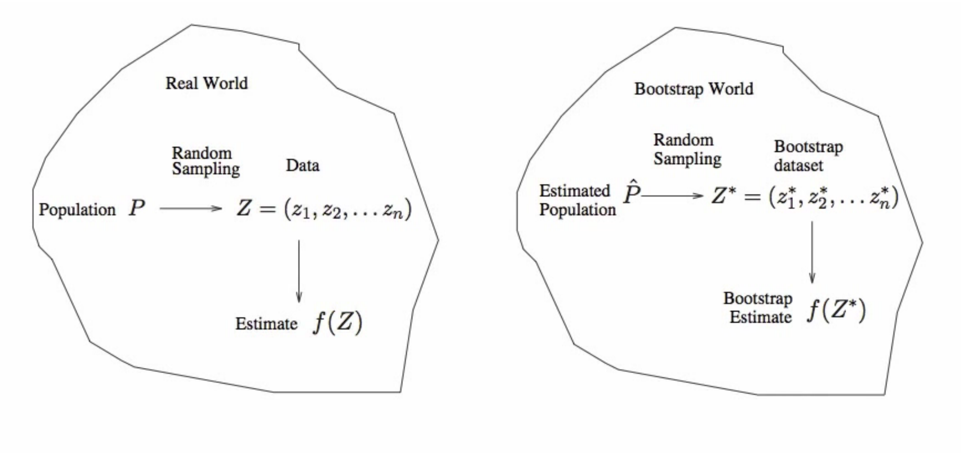

Real World
Random Sampling
Data
Population P
$Z = (z_1, z_2, \dots z_n)$
Estimate $f(Z)$
Bootstrap World
Random Sampling
Bootstrap dataset
Estimated Population $\hat{P}$
$Z^* = (z_1^*, z_2^*, \dots z_n^*)$
Bootstrap Estimate $f(Z^*)$

Figure 2: Sampling and resampling.

- The above interval is called a *Bootstrap Percentile* confidence interval. It is the simplest method for obtain a confidence interval from the bootstrap.

Compare Bootstrap and Cross Validation

- In CV, there is no overlap
- To estimate prediction error using the bootstrap, we could think about using each bootstrap dataset as our training sample, and the original samples as our validation set.
- But each bootstrap sample has significant overlap with the original data. About two-thirds of the original data points appear in each bootstrap sample.

5 Linear Model Selection and Regularization

5.1 Subset selection

The reason to alternate Least Square methods

- Prediction Accuracy: when $p > n$,, to control the variance.
- Model Interpretability: By setting the corresponding coefficient estimates to zero — we can obtain a model that is more easily interpreted. Feature selection.

Three major classes of methods

- *Subset Selection*: We identify a subset of the p predictors that we believe to be related to the response. We then fit the model using least squares on the reduced set of variables.
- *Shrinkage:*: We fit a model involving all p preditors, but the estimated coefficients are shrunken towards zero relative to the least squares estimates. The shrinkage aka regularization has the effect of reducing variance and can perform variable selection.
- *Dimension Reduction*. We project the p predictors into a M-dimensinoal subspace, where $M < p$. This is achieved by computing M different linear combinations, or projections of the variables. Then these M projections are used predictors to fit a linear regression model by least square.

Best Subset Selection

1. Let M_0 denote the *null model*, which contain no predictors. This model simply predicts the sample mean for each observation.

2. For $K = 1, 2, \dots p$:

   (a) Fit all $\binom{p}{k}$ models that contain exactly k predictors.

   (b) Pick the best among these $\binom{p}{k}$ models, and call it $\mathcal{M}_k$. Choose the best model having the smallest RSS, or largest R^2.

3. Select a single best frmo among $M_0, M_1, \dots, M_p$ using cross-validated prediction error, C_p (AIC), (BIC), or adjusted R^2.

Subset Selection applies to many methods, including least square regression, logistic regression, and so on. The deviance— negative two times the maximized log-likelihood—plays the role of RSS for a broader class of models.

Stepwise Selection

- Best subset selection does not apply with very large p. It leads to a large search space, and overfitting. And the complexity is $O(2^p)$.
- Forward stepwise selection begins with a model containing no predictors, and then adds predictors to the model, one-at-a-time, until all of the predictors are in the model.
- at each step the variable that gives the greatest additional improvement to the fit is added to the model.
- Complexity: $O(p^2)$

The other around is Backward Stepwise Selection.

- It searches through $1 + p(p+1)/2$ models, same as forward subset selection.
- Backward selection requires the number of sample n larger than the number of variables p, so that the full model can be fit. But forward does not have the requirement.

5.2 Some criterions

C_p, AIC, BIC and adjusted R^2

- They adjust the training error for the model size, and can be used to select among a set of models with different number of variables.
- Mallow's C_p

  $$C_p = \frac{1}{n}(\text{RSS} + 2d\hat{\sigma}^2),$$

  where d is the total number of parameters used and $\hat{sigma}^2$ is an estimate of the variance of the error ε associated with each response measurement. And $n > p$.

- The AIC criterion is defined for a large class of models fit by maximum likelihood:

  $$\text{AIC} = -2 \log L + 2 \cdot d,$$

  where L is the maximized value of the likelihood function for the estimated model.

- In the case of the linear model with Gaussian errors, maximium likelihood and least squares are the equivalent.
$$-2\log L = \mathrm{RSS}/\hat{\sigma}^2$$

Bayesian Information Criterion (BIC)

- $\mathrm{BIC} = \frac{1}{n}(\mathrm{RSS} + \log(n)d\hat{\sigma}^2)$.
- Like C_p, the BIC will tend to take on a small value for a model with a low test error, and so generally we select the model that has the lowest BIC value.
- BIC replaces the $2d\hat{\sigma}^2$ used by C_p with a $\log(n)d\hat{\sigma}^2$ term, where n is the number of observations.
- Since $\log n > 2$ for any $n > 7$, the BIC statistics generally places a heavier penalty on models with many variables, and hence results in the slection of smaller models than C_p.

Adjusted R^2

- For a least squares model with d variables, the adjusted R^2 statistic is calculated as
$$\text{Adjusted } R^2 = 1 - \frac{\mathrm{RSS}/(n-d-1)}{\mathrm{TSS}/(n-1)}.$$
where TSS is the total sum of squares.
- Unlike C_p, AIC, and BIC, for which a small value indicates a model with a low test error, a large value of adjusted R^2 indicateds a model with a small test error.
- Maximizing the adjusted R^2 is equivalent to minimizing $\mathrm{RSS}/(n-d-1)$. While RSS always decreases as the number of variables in the model inceases, $\mathrm{RSS}/(n-d-1)$ may increase or decrease, due to the presence of d in the denominator.
- unlike the R^2 statistic, the adjusted R^2 statstic pays a price for the inclusion of unnecessary variables in the model.

Validation and Cross-Validation

- The procedure has an adavantage over AIC, BIC, C_p and adjusted R^2, in that it provides a direct estimate of the test error, and does not require an estimate of the error variance σ^2.
- It can also be used in a wider range of model selection tasks, even in cases where it is hard to pinpoint the model degrees of freedom (the number of predictors in the model) or hard to estimate the error variance σ^2.

One-standard-error rule: We first calculate the standard error of the estimated test MSE for each model size, and the select the smallest model for which the estimated test error is within oen standard error of the lowest point on the curve.

5.3 Shrinkage Methods

Ridge regression and Lasso

- The subset selection methods use least squares to fit a linear model that contains a subset of predictors.
- Alternatively, we can fit a model containing all p predictors using a technique that constrains and regularizes the coefficient estimates, or shrinks the coefficient estimates towards zero.
- It may not be immediately obvious why such as contraint should improve the fit, but it turns out that shrinking the coefficient estimates can significantly reduce their variance.

Ridge Regression

$$\sum_{i=1}^{n}\left(y_i-\beta_0-\sum_{j=1}^{p}\beta_j x_{ij}\right)^2+\lambda\sum_{j=1}^{p}\beta_j^2=\text{RSS}+\lambda\sum_{j=1}^{p}\beta_j^2,$$

where $\lambda \geq 0$ is a tuning parameter, to be determined separately.

- As with least squares, ridge regression seeks coefficient estimates that fit the data well, by making the RSS small.
- However, the second term $\lambda\sum_j\beta_j^2$ called a shrinkage penalty, is small when $\beta_1,\ldots,\beta_p$ are close to zero, and so it has the effect of shrinking the estimates of β_j towards zero.
- The tuning parameter λ serves to control the relative impact of these two terms on the rgerssion coefficient estimates.
- Selecting a good value for λ is ciritical, cross validation is used for this.

Ridge Regression: scaling of predictors

- The standard least squares coefficient estimates are scale equivariant: multiplying X_j by a constant c simply leads to a scaling of the least squares coefficient estimates by a factor of $1/c$. In other words, regardless of how the jth predictor is scaled, $X_j\hat{\beta}_j$ will remain the same.
- In contrast, the ridge regression coefficient estimates can change substantially when multiplying a given predictor by a constant, due to the sum of squared coefficients term in the penalty part of the ridge regression objective function.
- It is best to apply ridge regression after standardizing the predictors, using the formula

$$\tilde{x}_{ij}=\frac{x_{ij}}{\frac{1}{n}\sum_{i=1}^{n}(x_{ij}-\bar{x}_j)^2}$$

One disadvantage of Ridge Regression is instead of involving a subset of variables in subset selection, ridge regression will include all p predictors in the final model.
The Lasso is a relatively new alternative to ridge regression that overcomes the disadvantage. The lasso coefficients, $\hat{\beta}_\lambda^L$ minimize the quantity

$$\sum_{i=1}^{n}\left(y_i-\beta_0-\sum_{j=1}^{p}\beta_j x_{ij}\right)+\lambda\sum_{j=1}^{p}|\beta_j|=\text{RSS}+\lambda\sum_{j=1}^{p}|\beta_j|.$$

In statistical parlance, the lasso uses an ℓ_1 penalty instead of an ℓ_2 penalty. The ℓ_1 norm of a coefficient vector β is given by $||\beta||_1=\sum|\beta_j|$.

- As with ridge regression, the lasso shrinks the coefficients estimates towards zero.
- In the case of lasso, the ℓ_1 penalty has the effect of forcing some of the coefficient estimates to be exactly equal to zero when the tuning paramter λ is suffciently large.
- Much like best subset selection, the lass performs variable selection.
- We say that the lasso yields sparse models — that is models that involve only a subset of the variables.
- As in ridge regression, selecting a good value of λ for the lasso is critical; cross-validation is the method of choice.

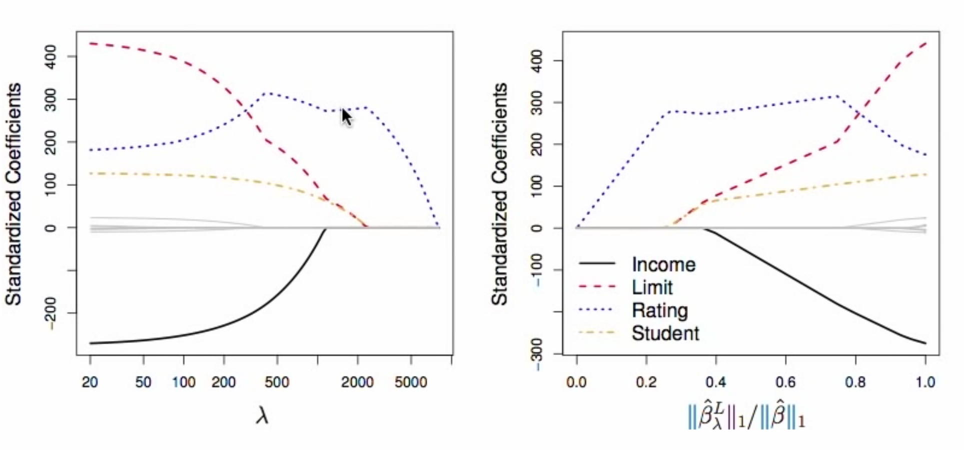


Figure 3: Lasso shrinks several variables towards zero.

We can see from the graph that by increasing λ, we can shrink some variables to exactly zero.
The Variable Selection Property of the Lasso
Why is it that the lasso, unlike ridge regressio, results in coefficent estimates that are exactly equal to zero? It is equivalent to say the lasso and ridge regression coefficient estimates solve the problems

$$\min_{\beta} \sum_{i=1}^{n} \left(y_i - \beta_0 - \sum_{j=1}^{p} \beta_j x_{ij} \right)^2 \tag{9}$$

$$\text{subject to } \sum_{j=1}^{p} |\beta_j| \leq s. \tag{10}$$

and

$$\min_{\beta} \sum_{i=1}^{n} \left(y_i - \beta_0 - \sum_{j=1}^{p} \beta_j x_{ij} \right)^2 \tag{11}$$

$$\text{subject to } \sum_{j=1}^{p} \beta_j^2 \leq s. \tag{12}$$

Selecting the tuning parameter for ridge regression and lasso using cross validation
We choose a grid of λ values, and compute the cross validation error rate for each value of λ. We then select the tuning parameter avlue for which the cross validation error is the smallest. $d \leq p$ but is unknown, so BIC, AIC and adjusted R^2 cannot be used.

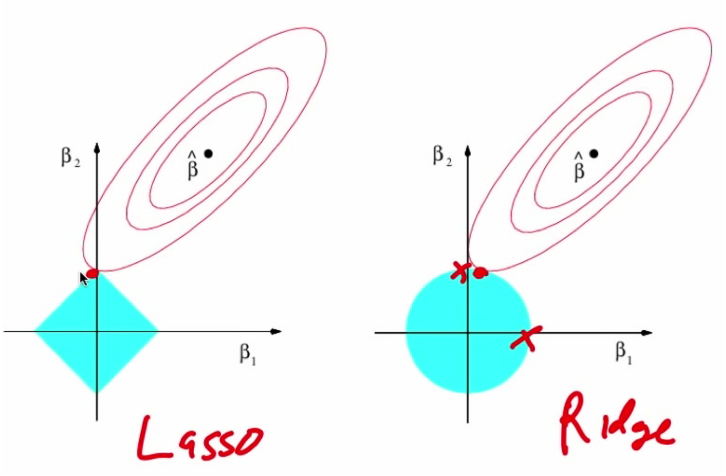


Figure 4: The lasso solution reaches the corner, which gives the sparsity.

5.4 Dimension Reduction Methods

- Let $Z_1, Z_2, \ldots, Z_M$ represent $M < p$ linear combinations of our original p predictors. That is

  $$Z_m = \sum_{j=1}^{p} \phi_{mj} X_j$$

  for some constants $\phi_{m1}, \ldots, \phi_{mp}$.

- We can then fit the linear regression model

  $$y_i = \theta_0 + \sum_{m=1}^{M} \theta_m z_{im} + \varepsilon_i, i = 1, \ldots, n$$

  using ordinary least squares.

- Note that in the second mode, the regression coefficients are given by $\theta_0, \theta_1, \ldots, \theta_M$. If the constants $\phi_{m1}, \ldots, \phi_{mp}$ are chosen wisely, the dimension reduction approaches can often outperform OLS regression.

- We do the transform as

  $$\sum_{m=1}^{M} \theta_m z_{im} = \sum_{m=1}^{M} \theta_m \sum_{j=1}^{p} \phi_{mj} x_{ij} = \sum_{j=1}^{p} \sum_{m=1}^{M} \theta_m \phi_{mj} x_{ij} = \sum_{j=1}^{p} \beta_j x_{ij}$$

  where

  $$\beta_j = \sum_{m=1}^{M} \theta_m \phi_{mj}.$$

- Dimension reduction serves to constrain the estimated coefficients, since now th ey must take the form as above.

Principal Component Regression

- PCR identifies linear combations or direction that best represent the predictors $X_1, \ldots, X_p$.

- These directions are identifies in an unsupervised way, since the response Y is not used to help determine th e principal component directions.

- The response does not supervise the identification of the principal component.

- There is no guarantee that the directions represent the predictors are the bes t directions for predicting the response.

Partial Least Squares (PLS)

- Unlike PCR, PLS identifies the new features in a supervised manner — it makes use of the response Y in order to identify new featuers that not only approximate the old features well, but are related to the response.

- Rougthly speaking, the PLS approach attempts to find directions that help explain both the response and the predictors.

PLS

- After standardizing the p predictors, PLS computes the first direction Z by setting each ϕ_{1j} equal to the coefficient from the simple linear regression of Y onto X_j.

- One can show this coefficient is proportional to the correlation between Y and X_j.

- In computing $Z_1 = \sum_{j=1}^{p} \phi_{1j} X_j$, PLS places the highest weight on the variables that are most strongly related to the response.

- Subsequent directions are found by taking residuals and then repeating the above prescription.

Polynomial Regression

- $$y_i = \beta_0 + \beta_1 x_i + \beta_2 x_i^2 + \beta_3 x_i^3 + \cdots + \beta_3 x_i^d + \varepsilon_i$$

- We look into the fitted function values at any value x_0:

$$\hat{f}(x_0) = \hat{\beta}_0 + \hat{\beta}_1 x_0 + \hat{\beta}_2 x_0^2 + \cdots + \hat{\beta}_k x_0^k$$

- Since $\hat{f}(x_0)$ is a linear function of the $\hat{\beta}_\ell$, we can get simple expression for pointwise-variances $\mathrm{Var}[\hat{f}(x_0)]$ at any value x_0.

- We either fix the degree d at some reasonble low value, or use cross validation.

- Nonlinear Logistic Regression

$$P(Y > 250 | X = x_i) = \frac{\exp(\beta_0 + \beta_1 x_i + \beta_2 x_i^2 + \cdots + \beta_d x_i^d)}{1 + \exp(\beta_0 + \beta_1 x_i + \beta_2 x_i^2 + \cdots + \beta_d x_i^d)}$$

- To get confidence intervals, compute upper and lower bounds *on the logit scale*, and then invert to get on probabiility scale.

- Can do separately on several variables — just stack the variables into one matrix, and separate out the pieces afterwards

- Caveat: polynomials have notrious tail behavior – very bad for extrapolation.

Step Functions
Another way of creating transformations of a variable — cut the variable into distinct regions. It is a local model. It is easy to work with, which creates a series of dummy variables representing each group.

Piecewise Polynomials

- Instead of a single polynomial in X over its whole domain, we can rather use different polynomials in regions defined by knots.

$$y_i = \begin{cases} \beta_{01} + \beta_{11}x_i + \beta_{21}x_i^2 + \beta_{31}x_i^3 + \varepsilon_i \text{ if } x_i < c; \\ \beta_{02} + \beta_{12}x_i + \beta_{22}x_i^2 + \beta_{32}x_i^3 + \varepsilon_i \text{ if } x_i < c; \end{cases}$$

- Better to add constraints to the polynomials, e.g. continuity

- Splines have the "maximum" amount of continuity

5.5 Nonline methods

Linear Splines
A linear spline with knots at $\varepsilon_k, k = 1, \dots, K$ is a piecewise linear polynomial continuous at each knot. We can represent this model as

$$y_i = \beta_0 + \beta_1 b_1(x_i) + \beta_2 b_2(x_i) + \cdots + \beta_{K+3} b_{K+3}(x_i) + \varepsilon_i,$$

where the b_k are basis functions.

$$b_1(x_i) = x_i \tag{13}$$

$$b_{k+1}(x_i) = (x_i - \xi_k)_+, \; k = 1, \dots, K \tag{14}$$

Here the $()_+$ means positive part, i.e.

$$(x_i - \xi_k)_+ = \begin{cases} x_i - \xi_k \text{ if } x_i > \xi_k; \\ 0 \text{ otherwise} \end{cases}$$

Cubic Splines A cubic spline with knots at ξ_k, $k = 1, \dots, K$ is piecewise cubic polynomial with continuous derivatives up to order 2 at each knot. We describe the model with truncated power basis functions

$$y = \beta_0 + \beta_1 b_1(x_i) + \beta_2 b_2(x_i) + \cdots + \beta_{K+1} b_{K+1}(x_i) + \varepsilon_i,$$

$$b_1(x_i) = x_i \tag{15}$$

$$b_2(x_i) = x_i^2 \tag{16}$$

$$b_3(x_i) = x_i^3 \tag{17}$$

$$b_{k+3}(x_i) = (x_i - \xi_k)_+^3, \; k = 1, \dots, K \tag{18}$$

$$(x_i - \xi_k)_+^3 = \begin{cases} (x_i - \xi_k)^3 \text{ if } x_i > \xi_k; \\ 0 \text{ otherwise} \end{cases}$$

Natural Cubic Splines

A natural cubic spline extraplates linearly beyond the boundary knots. This adds 4 extra contraints, and allow us to put more internal knots for the same degree of freedom as a regular cubic spline. Knot placement

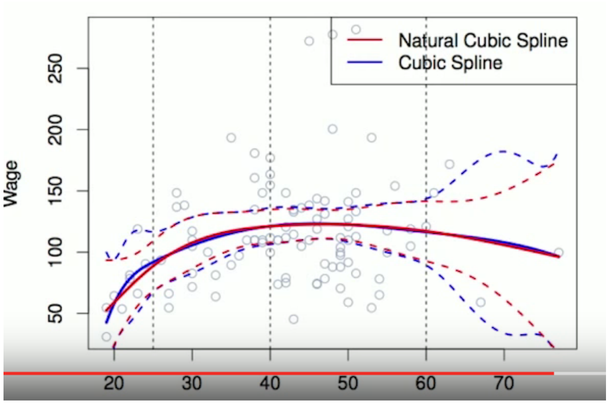


Figure 5: It shows the difference between Natural Cubic Spline and Cubic Spline.

- One strategy is to decide K, the number of knots, and then place them at appropriate quantiles of the observed X.
- A cubic spline with K knots has $K+4$ paramters or degree of freedom.
- A natural spline with K knots has K degrees of freedom.

Smoothing Splines
Consider fitting a smooth function to some data

$$\min_{g\in S} = \sum_{i=1}^{n}(y_i - g(x_i))^2 + \lambda \int g''(t)^2 dt$$

- The first term is RSS, and tries to make $g(x)$ match data at each x_i.
- The second term is a *roughness penalty* and controls how wiggly $g(x)$ is. It is modulated by the tuning parameter $\lambda \geq 0$.
  - The smaller λ, the more wiggly the function, eventually interpolating y_i when $\lambda = 0$.
  - As $\lambda \to \infty$, the function $g(x)$ becomes linear.
  - The solution is a natural cubic spline, with a knot at every unique value of x_i. The roughness peanlty still controls the roughness via λ.

Some details about Smoothing Spline

- Smoothing splines avoid the knot-selection issue, leaving single λ to be chosen.
- The vector of n fitted values can be written as $\hat{g}_\lambda = \mathbf{S}_\lambda \mathbf{y}$, where $\mathbf{S}_\lambda$ is a $n \times n$ matrix (determined by the x_i and λ)
- The effective degrees of feedom are given by

$$df_\lambda = \sum_{i=1}^{n}\{\mathbf{S}_\lambda\}_{ii}.$$

- We can specify df rather than λ.

Local Regression
With a sliding weight function, we fit separate linear fits over the range of X by weighed least squares.

Generalized Additive Models
Allows for flexible non-linearities in several variables, but retain the additive structure of linear models.

$$y_i = \beta_0 + f_1(x_{ij}) + f_2(x_{i2}) + \cdots + f_p(x_{ip}) + \varepsilon_i$$

GAMs for classification

$$\log\left(\frac{p(X)}{1-p(X)}\right) = \beta_0 + f_1(X_1) + f_2(X_2) + \cdots + f_p(X_p).$$

6 Tree-based methods

- It involves stratifying or segmenting the predictor space into a number of simple regions.
- Since the set of splitting rules used to segment the predictor psace can be summarized in a tree, these types of approaches are known as decision-tree methods.

6.1 Terminology for Trees

- In keeping with the tree analogy, the regions R_1, R_2, R_3 are known as terminal nodes.
- Decision trees are typically drawn upside down, in the sense that the leaves are at the bottom of the tree.
- The points along the tree where the predictor space is split are referred to as internal nodes

6.2 Tree-building process

- In theory, the regions could have any shape. However, we choose to divide the predictor space into high-dimensional rectangles, or boxes, for simplicity and for ease of interpretation of the resulting predictive model
- The goal is to find boxes $R_1, \ldots, R_J$ that minimize the RSS, given by

  $$\sum_{j=1}^{J} \sum_{i \in R_j} (y_i - \hat{y}_{R_j})^2.$$

  where $\hat{y}_{R_j}$ is the mean response for the training observations within the jth box, which is also one of the terminal leaves.
- It is computationally infeasible to consider every possible partition of the feature space into J boxes
- For this reason, we take a top-down, greedy approach that is know as recursive binary splitting
- The approach is top-down because it begins at the top of the tree and then succesively splits the predictor space; each split is indicated via two new branches further down on the tree
- It is greedy because at each step of the tree-building process, the best split is made at that particular step, rather than looking ahead and picking a split that will lead to a better tree in some future step.
- We predict the response for a given test observation using the mean of the training observations in the region to which that test observation belongs.

6.3 Pruning a tree

- Grow a very large tree T_0, and then prune it back in order to obtain a subtree.
- cost complexity pruning — also known as weakest link pruning is used to do this.
- We consider a sequence of trees indexed by a nonnegative tuning parameter α. For each value of α there corresponds a subtree $T \subset T_0$ such that

  $$\sum_{m=1}^{|T|} \sum_{i:x_i \in R_m} (y_i - \hat{y}_{R_m})^2 + \alpha|T|$$

  is as small as possible. Here $|T|$ indicates that the number of terminal nodes of the tree T, Rm is the rectangle (i.e. the subseet of predictor space) corresonding to the mth terminal node, and $\hat{y}_{R_m}$ is the mean of the training observations in R_m. The formulation is similar to the Lasso.
- The tuning paramter α controls a trade-off between the subtree's complexity and its fit to the training data.
- We select an optimal value $\hat{\alpha}$ using cross-validation.
- We then return to the full data set and obtain the subtree corresponding to $\hat{\alpha}$.

6.4 Classification Trees

- Very similar to a regression tree, except that it is used to predict a qualitative response rather than a quantitative one.
- For a classification tree, we predict that each observation belongs to the most commonly occurring class of training observations in the region to which it belongs.
- In the classification setting, RSS cannot be used as a criterion for making the binary splits
- A natural alternative to RSS is the classification error rate. this is simply the fraction fo the training observations in that region that do not belong to the most common class:

  $$E = 1 - \max_k(\hat{p}_{mk}).$$

  Here $\hat{p}_{mk}$ represents the proportion of training observation in the mth region that are from the kth class
- Classification error is not sufficiently sensitive for tree-growing, and in practice two other measures are preferable.
- The Gini index is defined by

  $$G = \sum_{k=1}^{K} \hat{p}_{mk}(1 - \hat{p}_{mk})$$

  a measure of total variance across the K classes. The Gini index takes on a small value if all of the $\hat{p}_{mk}$'s are close to zero or one
- For this reason the Gini index is referred to as a measure of node purity — a small value indicates that a node contains predominantly observations from a single class.

- An alternative to the Gini index is cross-entropy, given by

$$D = -\sum_{k=1}^{K} \hat{p}_{mk} \log \hat{p}_{mk}.$$

- It turns out that the Gini index and the cross-entropy are very similar numerically.

6.5 Bagging

- Bootstrap aggregation or bagging, is a general-purpose procedure for reducing the variance of a statistical learning method.
- Recall that given a set of n indepedent observations $Z_1, \ldots, Z_n$, each with variance σ^2, the variance of the mean $\bar{Z}$ of the observations is given by σ^2/n.
- In other words, averaging set of observations reduces variance.
- We generate B different bootstrapped trainnig data sets. We then train our method on the bth bootstrapped training set in order to get $\hat{f}^{*b}(x)$, the prediction at a point x. We then average all the prediction to obatin

$$\hat{f}_{bag}(x) = \frac{1}{B} \sum_{b=1}^{B} \hat{f}^{*b}(x)$$

- For classification trees: for each test observation, we record the class predicted by each of the B trees, and take a majority vote: the overall prediction is the most common occurring class among the B predictions.

Out-of-Bag Error Estimation

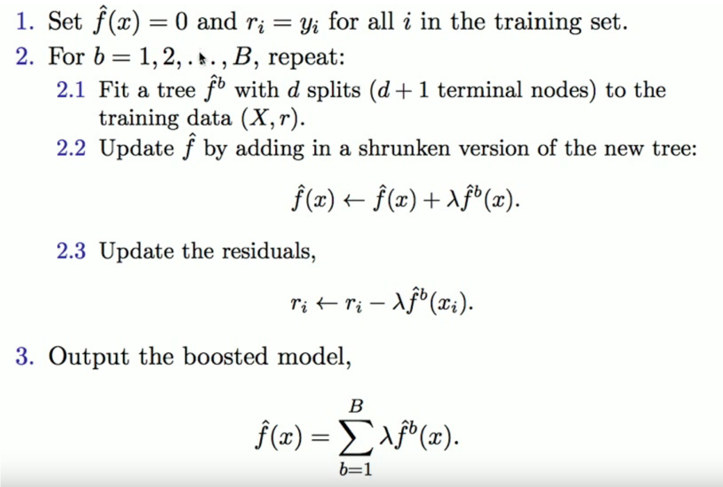
- There is a very straightforward way to estimate the test error of a bagged model.
- On can show that on average, each bagged tree makes use of around two-thirds of the observations.
- The remaining one-third of the observations not used to fit a given bagged tree are referred to as the out-of-bag (OOB) observations
- We can predict the response for the ith observation using each of the trees in which that observations was OOB. This will yield around $B/3$ predictions for the ith observation which we average.
- This estimate is essentially the LOO cross-validation erro for bagging, if B is large.

Random Forests

- RF provide an improvement over bagged trees by way of a small tweak that decorrelates the trees. This reduces the variance when we average the trees.
- As in bagging, we build a number of decision trees on bootstrapped training samples.
- But when building these decision trees, each time a split in a tree is considered, a random selection of m predictors is chosen as split candidates from the full set of p predictors. The split is allowed to use only one of those m predictors.
- A fresh selection of m predictors is taken at each split, and typicaly we choose $m \approx \sqrt{p}$ — that is, the number of predictors considered at each split is approxmately equal to the square root of the total number of predictors.

6.6 Boosting

Boosting for decision trees works in a similar way as bagging, except that trees are grown sequentially: each tree is grown using information from preivsouly grown trees. Boosting is a way of fitting an additive expansion in a set of elementary “basis” functions.



```
1. Set $\hat{f}(x) = 0$ and $r_i = y_i$ for all $i$ in the training set.
2. For $b = 1, 2, \ldots, B$, repeat:
    2.1 Fit a tree $\hat{f}^b$ with $d$ splits ($d + 1$ terminal nodes) to the
        training data $(X, r)$.
    2.2 Update $\hat{f}$ by adding in a shrunken version of the new tree:
            $\hat{f}(x) \leftarrow \hat{f}(x) + \lambda \hat{f}^b(x).$
    2.3 Update the residuals,
            $r_i \leftarrow r_i - \lambda \hat{f}^b(x_i).$
3. Output the boosted model,
            $\hat{f}(x) = \sum_{b=1}^{B} \lambda \hat{f}^b(x).$
```

Figure 6: Boosting algorithm.

The idea behind

- Unlike fitting a single large decision tree to the data, which amounts to fitting the data hard and potentially overfitting, the boosting approach instead learns slowly.
- Given the current model, we fit a decision tree to the residuals from the model. We then add this new decision tree into the fitted function in order to update the residuals.
- Each of these trees can be rather small, with just a few terminal nodes, determined by the parameter d in the algorithm.
- By fitting small trees to the residuals, we slowly improve $\hat{f}$ in areas where it does not perform well. The shrinkage parameter λ slows the process down even further, allowing more and different shaped trees to attack the residuals.

6.7 Gradient Boosting Decision Tree (GBDT)

The boosted tree model is a sum of trees,

$$f_M(x) = \sum_{m=1}^{M} T(x; \Theta_m)$$

At each step in the forward stagewise procedure one must solve

$$\hat{\Theta}_m = \arg\min_{\Theta_m} \sum_{i=1}^{N} L(y_i, f_{m-1}(x_i) + T(x_i; \Theta_m)).$$

for the region set and constants $\Theta_m = \{R_P ym, \gamma_{jm}\}_1^{J_m}$ of the next tree, given the current model $f_{m-1}(x)$.

7 Support Vector Machines

We try and find a plane that separates the classes in feature space.
If we cannot, we get creative in two ways:

- We soften what we mean by "separates", and
- We enrich and enlarge the feature space so that separation is possible.

7.1 What is a Hyperplane?

- A hyperplane in p dimension is a flat affine subspace of dimension $p-1$.
- In general the equation for a hyperplane has the form

$$\beta_0 + \beta_1 X_1 + \beta_2 X_2 + \cdots + \beta_p X_p = 0.$$

- In $p = 2$ dimensions a hyperplane is is a line
- If $\beta_0 = 0$, then the hyperplane goes through the origin, otherwise not.
- The vector $\beta = (\beta_1, \beta_2, \dots \beta_p)$ is called the normal vector — it points in a direction orthogonal to the surface of a hyperplane.

7.2 Maximal Margin Classifier

Among all separating hyperplanes, find the one that makes the biggest gap or margin between the two classes.
Constrained optimization problem

$$\underset{\beta_0,\beta_1,\dots,\beta_p}{\text{maximize}} M$$

subject to $\sum_{j=1}^{p} \beta_j^2 = 1,, y_i(\beta_0 + \beta_1 x_{i1} + \cdots + \beta_p x_{ip}) \geq M$ for all $i = 1, \dots, N$. The data is separable when $N < p$, such as the genome data. When non-separable, the support vector classifier maximizes a soft margin.
$\underset{\beta_0,\beta_1,\dots,\beta_p,\varepsilon_1,\dots\varepsilon_n}{\text{maximize}} \; M$ subject to $\sum_{j=1}^{p} \beta_j^2 = 1$, $y_i(\beta_0 + \beta_1 x_{i1} + \cdots + \beta_p x_{ip}) \geq M(1 - \varepsilon_i)$, $\varepsilon \geq 0$, $\sum_{i=1}^{n} \varepsilon_i \leq C$.
ε is a slack which allows for some errors inside the margins, C is a regularization parameter, which is a budget of ε. Increasing C makes the margin "softer," so that the orientation of the separating hyperplane is influenced by more points.
Note. Lasso and Ridge Regression and SVMs treat the samples equally, so they should be standardized beforehand.
Feature Expansion

- Enlarge the space of features by including transformations; e.g. $X_1^2, X_1^3, X_1X_2, X_1X_2^2, \dots$. Hence go from a p dimensional space to a $M > p$ dimensional space.
- Fit a support-vector classifier in the enlarged space.
- This results in non-linear decision boundaries in the original space.
- For example, suppose we use $(X_1, X_2, X_1^2, X_2^2, X_1X_2)$ instead of just (X_1, X_2). Then the decision boundary would be of the form

$$\beta_0 + \beta_1 X_1 + \beta_2 X_2 + \beta_3 X_1^2 + \beta_4 X_2^2 + \beta_5 X_1 X_2 = 0$$

This leads to nonlinear decision boundaries in the original space (Cubic Polynomials). It is linear in the new variable space, which results in a linear boundary in the high dimensional space. But nonlinear in the original space. In the lower dimensional space, however, these are conic sections of a quadratic polynomial.

Inner products and support vectors

- The linear support vector classifier can be represented as

$$f(x) = \beta_0 + \sum_{i=1}^{n} \alpha_i \langle x, x_i \rangle \text{ — } n \textit{ parameters}.$$

- To estimate the parameters $\alpha_1, \ldots, \alpha_n$ and β_0, all we need are the $\binom{n}{2}$ inner products $\langle x_i, x_{i'} \rangle$ between all pairs of training observations.

- It turns out that most of the $\hat{\alpha}_i$ can be zero:

$$f(x) = \beta_0 + \sum_{i \in \mathcal{S}} \hat{\alpha}_i \langle x, x_i \rangle,$$

  where $\mathcal{S}$ is the support set of indices i such that $\hat{\alpha}_i > 0$. It is a sparsity in the data space.

7.3 Regularization and reproducing kernel Hilbert spaces

A generalized class of regularization problems has the form

$$\min_{f \in \mathcal{H}} \left[\sum_{i=1}^{N} L(y_i, f(x_i)) + \lambda J(f) \right]$$

where $L(y, f(x))$ is a loss function, $J(f)$ is a penalty functional and $\mathcal{H}$ is a space of functions which $J(f)$ is defined.

An important subclass of problems of the form are generated by a postive definite kernel $K(x,y)$, and the corresponding space of functions $\mathcal{H}_K$ is called a *reproducing kernel Hilbert space* (RKHS). The penalty functional J is defined in terms of the kernel as well. Let $x, y \in \mathbb{R}^p$. We consider the space of functions generated by the linear span of $\{K(\cdot, y), y \in \mathbb{R}^p\}$; i.e. arbitrary linear combinations of the form $f(x) = \sum_m \alpha_m K(x, y_m)$, where each kernel term is viewed as a function of the first argument, and indexed by the second. Suppose that K has an eigen-expansion

$$K(x,y) = \sum_{i=1}^{\infty} \gamma_i \phi_i(x) \phi_i(y),$$

with $\gamma_i \geq 0$, $\sum_{i=1}^{\infty} \gamma_i^2 < \infty$. Elements of $\mathcal{H}_K$ have an expansion in terms of these eigen-functions,

$$f(x) = \sum_{i=1}^{\infty} c_i \phi_i(x).$$

with the constraint that

$$\|f\|_{\mathcal{H}_K}^2 = \sum_{i=1}^{\infty} c_i^2 / r_i < \infty,$$

where $\|f\|_{\mathcal{H}_K}$ is the norm induced by K. The penalty function for the space $\mathcal{H}_K$ is defined to be the squared norm $J(f) = \|f\|_{\mathcal{H}_K}^2$. The quantity $J(f)$ can be interpreted as a generalized ridge penalty, where functions with large eigenvalues in the expansion get penalized less and vice versa.

Kernels and Support Vector Machines

- If we can compute inner-products between observations, we can fit a SV classifier. It can be quite abstract.

- Some special *kernel functions* can do this for us. E.g.

  $$K(x_i, x_{i'}) = \left(1 + \sum_{j=1}^{p} x_{ij} x_{i'j}\right)^d$$

  computes the inner-products needed for d dimensional polynomials — $\binom{p+d}{d}$ basis functions.

- The solution has the form

  $$f(x) = \beta_0 + \sum_{i \in \mathcal{S}} \hat{\alpha}_i K(x, x_i).$$

  Radial Kernel

  $$K(x_i, x_{i'}) = \exp(-\gamma \sum_{j=1}^{p} (x_{ij} - x_{i'j})^2),$$

  It has an implicit feature space, and is very high dimesnional, It controls variance by squashing down most dimensions severely.

  More than 2 classes

  OVA: One versus All. Fit K different 2-class SVM classifiers $\hat{f}_k(x)$, k=1,...,K; each class versus the rest. Classify x^* to the class for which $\hat{f}_k(x^*)$ is largest.

  OVO: One versus One. Fit all $\binom{K}{2}$ pairwise classifiers $\hat{f}_{k\ell}(x)$. Classify x^* to the class that wins the most pairwise competitions.

7.4 Support Vector Machines vs Logistic Regression

With $f(X) = \beta_0 + \beta_1 X_1 + \cdots + \beta_p X_p$ can rephrase support vector classifier optimization as

$$\underset{\beta_0, \beta_1, \ldots, \beta_p}{\text{minimize}} \left(\max[0, 1 - y_i f(x_i)] + \lambda \sum_{j=1}^{p} \beta_j^2 \right)$$

This has the form loss plus penalty. This loss is known as the hinge loss, which is very similar to “loss”

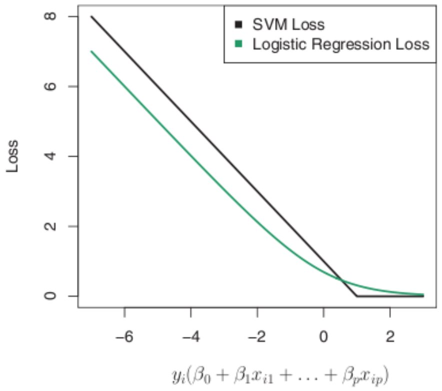


Figure 7: SVMs vs Logistic Regression.

in logistic regression (negative log-likelihood).

Which one to use

- When clases are nearly separable, SVM and LDA do better than LR.
- When not, LR (with ridge penalty) and SVM perform similarly.
- If you wish to etimate probabilities, LR is the choice.
- For nonlinear boundaries, kernel SVMs are popular. Can use kernels with LR and LDA as well, but computations are more expensive.

8 Unsupervised learning

8.1 PCA

The principal component direction $\phi_1, \phi_2, \phi_3 \dots$ are the ordered sequence of right singular vectors of the matrix $\mathbf{X}$, and the variances of the components are $\frac{1}{n}$ times the squares of the singular values. There are at most $\min(n-1, p)$ principal components.

Hyperplane on PCA and linear regression. For linear regression, we measure the distance from the label y to the point in the hyperplane. By contrast, PCA finds the shortest distance from the data points to the hyperplane, and the distance is perpendicular to the hyperplane. In other words, we find a hyperplane that passes through the middle of the data points, We compute the distance from the data points to the hyperplane and sum the sqauress of the distance. We want the hyperplane that gets closest to the data.

Scaling of the variables matters — If the varaibles are in different units, scaling each to have standard deviation equal to one is recommended.

- The first principal component of a set of features $X_1, X_2, \dots, X_p$ is the normalized lienar combinaton of the features
$$Z_1 = \phi_{11}X_1 + \phi_{21}X_2 + \cdots + \phi_{p1}X_p$$
that has the largest variance. By normalized, we mean that $\sum_{j=1}^{p} \phi_{j1}^2 = 1$.
- We refer to the elements $\phi_{11}, \dots, \phi_{p1}$ as the loadings of the first principal component; together, the loadings make up the principal component loading vector, $\phi_1 = (\phi_{11}\phi_{21}\dots\phi_p 1)^\top$.
- We constrain the loadings so that theri sum of squares is equal to one, since otherwise setting these elements to be arbitrarily large in absolute value could result in an arbitrarily large variance.

Proportion Variance Explained

- To understand the strength of each PCA component, we are interested in knowing the proportion of variance explained (PVE) by each one.
- The total variance present in data set (assuming that the varaibles have been centered to have mean zero) is defined as
$$\sum_{j=1}^{p} \mathrm{Var}(X_j) = \sum_{j=1}^{p} \frac{1}{n} \sum_{i=1}^{n} x_{ij}^2$$
and the variance explained by the mth principal component is
$$\mathrm{Var}(Z_m) = \frac{1}{n} \sum_{i=1}^{n} z_{im}^2$$
- It can be shown that $\sum_{j=1}^{p} \mathrm{Var}(X_j) = \sum_{m=1}^{M} \mathrm{Var}(Z_m)$, with $M = \min(n-1, p)$.

- the PVE of the *m*th principal component is given by the positive quantity between 0 and 1

$$\frac{\sum_{i=1}^{n} z_{im}^2}{\sum_{j=1}^{p} \sum_{j=1}^{n} x_{ij}^2}$$

- The PVEs sum to one. We sometimes display the cumulative PVEs.

To select the number of components, we could use cross-validation to find the number of components used in regression. We cannot use the cross-validation directly due to the lack of reponse.

8.2 Clustering

K-means

- The idea behind K-means clustering is a good clustering is one for which the within-cluster variation is as small as possible.
- The within-cluster variation for cluster C_k is a measure $WCV(C_k)$ of the amount by which the observations within a cluster differ from each other.
- We want to solve the problem

$$\underset{C1,\ldots,C_k}{\text{minimize}} \left\{ \sum_{k=1}^{K} WCV(C_k) \right\} = \underset{C_1,\ldots,C_K}{\text{minimize}} \left\{ \sum_{k=1}^{K} \frac{1}{|C_k|} \sum_{i,i' \in C_k} \sum_{j=1}^{p} (x_{ij} - x_{i'j})^2 \right\}. \tag{19}$$

- The algorithm is guaranteed to decrease the value of the objective at each step.

$$\frac{1}{|C_k|} \sum_{i,i' \in C_k} \sum_{j=1}^{p} (X_{ij} - x_{i'j})^2 = 2 \sum_{i \in C_k} \sum_{j=1}^{p} (x_{ij} - \bar{x}_{kj})^2.$$

  where $\bar{x}_{kj} = \frac{1}{|C_k|} \sum_{i \in C_k x_{ij}}$ is the mean for feature j in cluster C_k. However, it is not guaranteed to give the global minimum.

In hierarchical clustering, we do not know in advance how many clusters we want; in fact, we end up with a tree-like visual representation of the observations, called a dendrogram, that allows us to view at once the clusterings obtained for each possible number of clusters, from 1 to n.
In case of hierarchical clustering,

- What dissimilarity measure should be used
- What type of linkage should be used

Some engineering can also be done to select the samples. In the breast cancer microarray example, they select 500 intrinsic genes out of 8000 genes, which have the smallest within/between variation. The intrinsic genes varies a lot between women but little within women.

9 Predictive Analytics for Data Mining

- In data mining applications, usually only a small fraction of the large number of predictor variables that have been included in the analysis are actually relevant to prediction.
- Unlike many applications such as pattern recognition, there is seldom reliable domain knowledge to help create especially relevant features and/or filter out the irrelevant ones, the inclusion of which dramatically degrades the performance of many methods.
- It is also desirable to have information providing qualitative understanding of the relationship between joint values of the input variables and the resulting predicted response value.

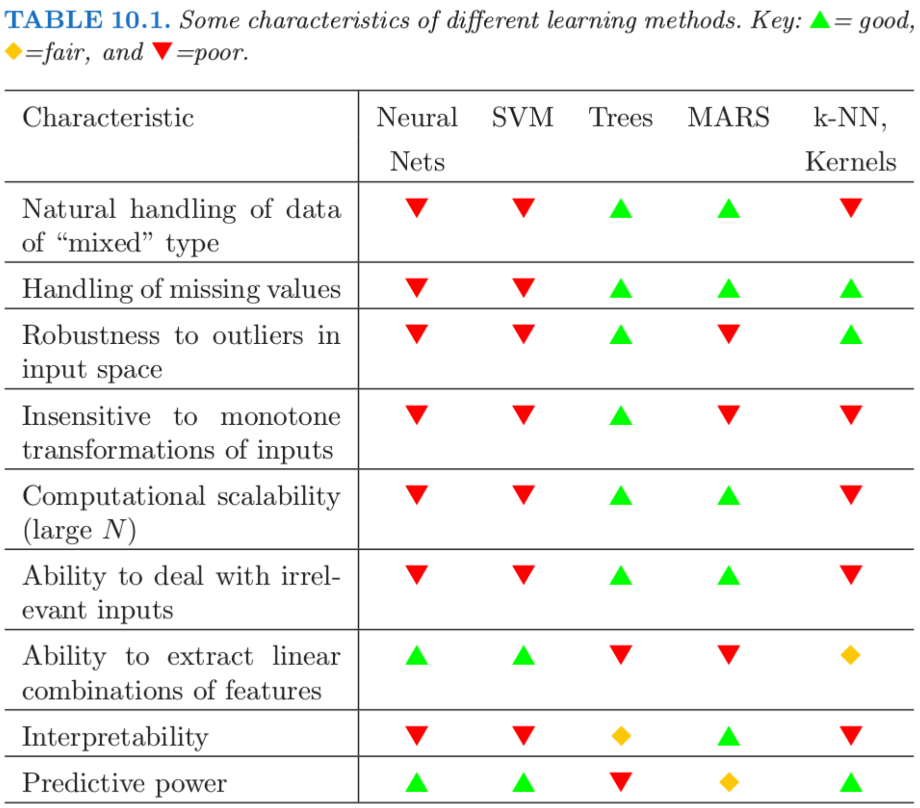


TABLE 10.1. *Some characteristics of different learning methods. Key:* ▲= *good,* ◆=*fair, and* ▼=*poor.*

Characteristic	Neural Nets	SVM	Trees	MARS	k-NN, Kernels
Natural handling of data of “mixed” type	▼	▼	▲	▲	▼
Handling of missing values	▼	▼	▲	▲	▲
Robustness to outliers in input space	▼	▼	▲	▼	▲
Insensitive to monotone transformations of inputs	▼	▼	▲	▼	▼
Computational scalability (large N)	▼	▼	▲	▲	▼
Ability to deal with irrelevant inputs	▼	▼	▲	▲	▼
Ability to extract linear combinations of features	▲	▲	▼	▼	◆
Interpretability	▼	▼	◆	▲	▼
Predictive power	▲	▲	▼	◆	▲

Figure 8: Some properties in predictive analytics.