

FRE6871 R in Finance

Lecture#5, Fall 2022

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October 3, 2022



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Multivariate Linear Regression

A *multivariate* linear regression model with k *predictors* x_j , is defined by the formula:

$$y_i = \alpha + \sum_{j=1}^k \beta_j x_{i,j} + \varepsilon_i$$

α and β are the unknown regression coefficients, with α a scalar and β a vector of length k .

The *residuals* ε_i are assumed to be normally distributed $\phi(0, \sigma_\varepsilon)$, independent, and stationary.

The data consists of n observations, with each observation containing k *predictors* and one *response* value.

The *response vector* y , the *predictor vectors* x_j , and the *residuals* ε are vectors of length n .

The k *predictors* x_j form the columns of the (n, k) -dimensional *predictor matrix* \mathbb{X} .

The *multivariate regression* model can be written in vector notation as:

$$y = \alpha + \mathbb{X}\beta + \varepsilon = y_{fit} + \varepsilon$$

$$y_{fit} = \alpha + \mathbb{X}\beta$$

Where y_{fit} are the *fitted values* of the model.

```
> # Define predictor matrix
> nrows <- 100
> ncols <- 5
> set.seed(1121) # initialize random number generator
> predictor <- matrix(rnorm(nrows*ncols), ncol=ncols)
> # Add column names
> colnames(predictor) <- paste0("col", 1:ncols)
> # Define the predictor weights
> weights <- sample(3:(ncols+2))
> # Response equals weighted predictor plus random noise
> noise <- rnorm(nrows, sd=5)
> response <- (-3 + 2*predictor %*% weights + noise)
```

Solution of Multivariate Regression

The *Residual Sum of Squares* (*RSS*) is defined as the sum of the squared *residuals*:

$$RSS = \varepsilon^T \varepsilon = (y - y_{fit})^T (y - y_{fit}) = (y - \alpha + \mathbb{X}\beta)^T (y - \alpha + \mathbb{X}\beta)$$

The *OLS* solution for the regression coefficients is found by equating the *RSS* derivatives to zero:

$$RSS_{\alpha} = -2(y - \alpha - \mathbb{X}\beta)^T \mathbf{1} = 0$$

$$RSS_{\beta} = -2(y - \alpha - \mathbb{X}\beta)^T \mathbb{X} = 0$$

The solutions for α and β are given by:

$$\alpha = \bar{y} - \bar{\mathbb{X}}\beta$$

$$RSS_{\beta} = -2(\hat{y} - \hat{\mathbb{X}}\beta)^T \hat{\mathbb{X}} = 0$$

$$\hat{\mathbb{X}}^T \hat{y} - \hat{\mathbb{X}}^T \hat{\mathbb{X}}\beta = 0$$

$$\beta = (\hat{\mathbb{X}}^T \hat{\mathbb{X}})^{-1} \hat{\mathbb{X}}^T \hat{y} = \hat{\mathbb{X}}^{inv} \hat{y}$$

Where \bar{y} and $\bar{\mathbb{X}}$ are the column means, and $\hat{\mathbb{X}} = \mathbb{X} - \bar{\mathbb{X}}$ and $\hat{y} = y - \bar{y} = \hat{\mathbb{X}}\beta + \varepsilon$ are the de-meaned variables.

The matrix $\hat{\mathbb{X}}^{inv}$ is the generalized inverse of the de-meaned *predictor matrix* $\hat{\mathbb{X}}$.

The matrix $\mathbb{C} = \hat{\mathbb{X}}^T \hat{\mathbb{X}} / (n - 1)$ is the *covariance matrix* of the matrix \mathbb{X} , and it's invertible only if the columns of \mathbb{X} are linearly independent.

```
> # Perform multivariate regression using lm()
> regmod <- lm(response ~ predictor)
> # Solve multivariate regression using matrix algebra
> # Calculate de-meaned predictor matrix and response vector
> predzm <- t(t(predictor) - colMeans(predictor))
> # predictor <- apply(predictor, 2, function(x) (x-mean(x)))
> respzm <- response - mean(response)
> # Calculate the regression coefficients
> betas <- drop(MASS::ginv(predzm) %*% respzm)
> # Calculate the regression alpha
> alpha <- mean(response) - sum(colSums(predictor)*betas)/nrows
> # Compare with coefficients from lm()
> all.equal(coef(regmod), c(alpha, betas), check.attributes=FALSE)
[1] TRUE
> # Compare with actual coefficients
> all.equal(c(-1, weights), c(alpha, betas), check.attributes=FALSE)
[1] "Mean relative difference: 1.07"
```

Multivariate Regression in Homogeneous Form

We can add an extra unit column to the *predictor matrix* \mathbb{X} to represent the intercept term, and express the *linear regression formula in homogeneous form*:

$$y = \mathbb{X}\beta + \varepsilon$$

Where the *regression coefficients* β now contain the intercept α : $\beta = (\alpha, \beta_1, \dots, \beta_k)$, and the *predictor matrix* \mathbb{X} has $k + 1$ columns and n rows.

The *OLS* solution for the β coefficients is found by equating the *RSS* derivative to zero:

$$RSS_{\beta} = -2(y - \mathbb{X}\beta)^T \mathbb{X} = 0$$

$$\mathbb{X}^T y - \mathbb{X}^T \mathbb{X} \beta = 0$$

$$\beta = (\mathbb{X}^T \mathbb{X})^{-1} \mathbb{X}^T y = \mathbb{X}_{inv} y$$

The matrix $\mathbb{X}_{inv} = (\mathbb{X}^T \mathbb{X})^{-1} \mathbb{X}^T$ is the generalized inverse of the *predictor matrix* \mathbb{X} .

The coefficients β can be interpreted as the projections of the *response vector* y onto the columns of the *predictor matrix* \mathbb{X} .

The *predictor matrix* \mathbb{X} maps the *regression coefficients* β into the *response vector* y .

The generalized inverse of the *predictor matrix* \mathbb{X}_{inv} maps the *response vector* y into the *regression coefficients* β .

```
> # Add intercept column to predictor matrix
> predictor <- cbind(rep(1, NROW(predictor)), predictor)
> ncols <- NCOL(predictor)
> # Add column name
> colnames(predictor)[1] <- "intercept"
> # Calculate generalized inverse of the predictor matrix
> invpred <- MASS::ginv(predictor)
> # Calculate the regression coefficients
> betas <- invpred %*% response
> # Perform multivariate regression without intercept term
> regmod <- lm(response ~ predictor - 1)
> all.equal(drop(betas), coef(regmod), check.attributes=FALSE)
[1] TRUE
```

The Residuals of Multivariate Regression

The *multivariate regression* model can be written in vector notation as:

$$y = X\beta + \varepsilon = y_{fit} + \varepsilon$$

$$y_{fit} = X\beta$$

Where y_{fit} are the *fitted values* of the model.

The *residuals* are equal to the *response vector* minus the *fitted values*: $\varepsilon = y - y_{fit}$.

The *residuals* ε are orthogonal to the columns of the *predictor matrix* X (the *predictors*):

$$\varepsilon^T X = (y - X(X^T X)^{-1} X^T y)^T X =$$

$$y^T X - y^T X (X^T X)^{-1} X^T X = y^T X - y^T X = 0$$

Therefore the *residuals* are also orthogonal to the *fitted values*: $\varepsilon^T y_{fit} = \varepsilon^T X\beta = 0$.

Since the first column of the *predictor matrix* X is a unit vector, the *residuals* ε have zero mean: $\varepsilon^T \mathbf{1} = 0$.

```
> # Calculate fitted values from regression coefficients
> fittedv <- drop(predictor %*% betas)
> all.equal(fittedv, regmod$fitted.values, check.attributes=FALSE)
[1] TRUE
> # Calculate the residuals
> residuals <- drop(response - fittedv)
> all.equal(residuals, regmod$residuals, check.attributes=FALSE)
[1] TRUE
> # Residuals are orthogonal to predictor columns (predictors)
> sapply(residuals %*% predictor, all.equal, target=0)
[1] TRUE TRUE TRUE TRUE TRUE TRUE
> # Residuals are orthogonal to the fitted values
> all.equal(sum(residuals*fittedv), target=0)
[1] TRUE
> # Sum of residuals is equal to zero
> all.equal(sum(residuals), target=0)
[1] TRUE
```

The Influence Matrix of Multivariate Regression

The vector $y_{fit} = \mathbb{X}\beta$ are the *fitted values* corresponding to the *response vector* y :

$$y_{fit} = \mathbb{X}\beta = \mathbb{X}(\mathbb{X}^T\mathbb{X})^{-1}\mathbb{X}^T y = \mathbb{X}\mathbb{X}_{inv}y = \mathbb{H}y$$

Where $\mathbb{H} = \mathbb{X}\mathbb{X}_{inv} = \mathbb{X}(\mathbb{X}^T\mathbb{X})^{-1}\mathbb{X}^T$ is the *influence matrix* (or *hat matrix*), which maps the *response vector* y into the *fitted values* y_{fit} .

The *influence matrix* \mathbb{H} is a projection matrix, and it measures the changes in the *fitted values* y_{fit} due to changes in the *response vector* y .

$$\mathbb{H}_{ij} = \frac{\partial y_i^{fit}}{\partial y_j}$$

The square of the *influence matrix* \mathbb{H} is equal to itself (it's idempotent): $\mathbb{H}\mathbb{H}^T = \mathbb{H}$.

```
> # Calculate the influence matrix
> influencem <- predictor %*% invpred
> # The influence matrix is idempotent
> all.equal(influencem, influencem %*% influencem)
[1] TRUE
> # Calculate fitted values using influence matrix
> fittedv <- drop(influencem %*% response)
> all.equal(fittedv, regmod$fitted.values, check.attributes=FALSE)
[1] TRUE
> # Calculate fitted values from regression coefficients
> fittedv <- drop(predictor %*% betas)
> all.equal(fittedv, regmod$fitted.values, check.attributes=FALSE)
[1] TRUE
```

Multivariate Regression With de-Meaned Variables

The *multivariate regression* model can be written in vector notation as:

$$y = \alpha + \mathbb{X}\beta + \varepsilon$$

The intercept α can be substituted with its solution: $\alpha = \bar{y} - \bar{\mathbb{X}}\beta$ to obtain the regression model with de-meaned response and predictor matrix:

$$y = \bar{y} - \bar{\mathbb{X}}\beta + \mathbb{X}\beta$$

$$\hat{y} = \mathbb{X}\beta + \varepsilon$$

The regression model with a de-meaned *predictor matrix* produces the same *fitted values* (only shifted by their mean) and *residuals* as the original regression model, so it's equivalent to it. has the same influence matrix, and

But the de-meaned regression model has a different *influence matrix*, which maps the de-meaned *response vector* \hat{y} into the de-meaned *fitted values* \hat{y}_{fit} .

```
> # Calculate zero mean fitted values
> predzm <- t(t(predictor) - colMeans(predictor))
> fitted_zm <- drop(predzm %*% betas)
> all.equal(fitted_zm,
+   regmod$fitted.values - mean(response),
+   check.attributes=FALSE)
[1] TRUE
> # Calculate the residuals
> respzm <- response - mean(response)
> residuals <- drop(respzm - fitted_zm)
> all.equal(residuals, regmod$residuals,
+   check.attributes=FALSE)
[1] TRUE
> # Calculate the influence matrix
> influence_zm <- predzm %*% MASS::ginv(predzm)
> # Compare the fitted values
> all.equal(fitted_zm,
+   drop(influence_zm %*% respzm),
+   check.attributes=FALSE)
[1] TRUE
```

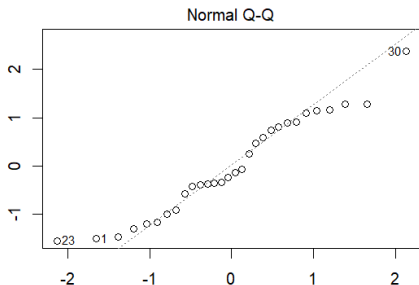
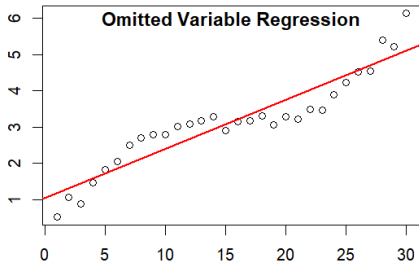
Omitted Variable Bias

Omitted Variable Bias occurs in a regression model that omits important predictors.

The parameter estimates are biased, even though the t -statistics, p -values, and R -squared all indicate a statistically significant regression.

But the Durbin-Watson test shows that the residuals are autocorrelated, which means that the regression coefficients may not be statistically significant (different from zero).

```
> library(lmtest) # Load lmtest
> # Define predictor matrix
> predictor <- 1:30
> omitv <- sin(0.2*1:30)
> # Response depends on both predictors
> response <- 0.2*predictor + omitv + 0.2*rnorm(30)
> # Mis-specified regression only one predictor
> model_ovb <- lm(response ~ predictor)
> modelsum <- summary(regmod_ovb)
> modelsum$coeff
> modelsum$r.squared
> # Durbin-Watson test shows residuals are autocorrelated
> lmtest::dwtest(regmod_ovb)
> # Plot the regression diagnostic plots
> x11(width=5, height=7)
> par(mfrow=c(2,1)) # Set plot panels
> par(mar=c(3, 2, 1, 1), oma=c(1, 0, 0, 0))
> plot(response ~ predictor)
> abline(regmod_ovb, lwd=2, col="red")
> title(main="Omitted Variable Regression", line=-1)
> plot(regmod_ovb, which=2, ask=FALSE) # Plot just Q-Q
```



Regression Coefficients as *Random Variables*

The *residuals* $\hat{\varepsilon}$ can be considered to be *random variables*, with expected value equal to zero $\mathbb{E}[\hat{\varepsilon}] = 0$, and variance equal to σ_{ε}^2 .

The variance of the *residuals* is equal to the expected value of the squared *residuals* divided by the number of *degrees of freedom*:

$$\sigma_{\varepsilon}^2 = \frac{\mathbb{E}[\varepsilon^T \varepsilon]}{d_{\text{free}}}$$

Where $d_{\text{free}} = (n - k)$ is the number of *degrees of freedom* of the *residuals*, equal to the number of observations n , minus the number of *predictors* k (including the intercept term).

The *response vector* y can also be considered to be a *random variable* \hat{y} , equal to the sum of the deterministic *fitted values* y_{fit} plus the random *residuals* $\hat{\varepsilon}$:

$$\hat{y} = \mathbb{X}\beta + \hat{\varepsilon} = y_{\text{fit}} + \hat{\varepsilon}$$

The *regression coefficients* β can also be considered to be *random variables* $\hat{\beta}$:

$$\begin{aligned}\hat{\beta} &= \mathbb{X}_{\text{inv}} \hat{y} = \mathbb{X}_{\text{inv}} (y_{\text{fit}} + \hat{\varepsilon}) = \\ &= (\mathbb{X}^T \mathbb{X})^{-1} \mathbb{X}^T (\mathbb{X}\beta + \hat{\varepsilon}) = \beta + \mathbb{X}_{\text{inv}} \hat{\varepsilon}\end{aligned}$$

Where β is equal to the expected value of $\hat{\beta}$:
 $\beta = \mathbb{E}[\hat{\beta}] = \mathbb{X}_{\text{inv}} y_{\text{fit}} = \mathbb{X}_{\text{inv}} y$.

```
> # Regression model summary
> modelsum <- summary(regmod)
> # Degrees of freedom of residuals
> nrow <- NROW(predictor)
> ncol <- NCOL(predictor)
> degf <- (nrow - ncol)
> all.equal(degf, modelsum$df[2])
[1] TRUE
> # Variance of residuals
> residvar <- sum(residuals^2)/degf
```

Covariance Matrix of the Regression Coefficients

The *covariance matrix* of the *regression coefficients* $\hat{\beta}$ is given by:

$$\begin{aligned}\sigma_{\beta}^2 &= \frac{\mathbb{E}[(\hat{\beta} - \beta)(\hat{\beta} - \beta)^T]}{d_{\text{free}}} = \\ \frac{\mathbb{E}[\mathbb{X}_{\text{inv}} \hat{\varepsilon} (\mathbb{X}_{\text{inv}} \hat{\varepsilon})^T]}{d_{\text{free}}} &= \frac{\mathbb{E}[\mathbb{X}_{\text{inv}} \hat{\varepsilon} \hat{\varepsilon}^T \mathbb{X}_{\text{inv}}^T]}{d_{\text{free}}} = \\ \frac{(\mathbb{X}^T \mathbb{X})^{-1} \mathbb{X}^T \mathbb{E}[\hat{\varepsilon} \hat{\varepsilon}^T] \mathbb{X} (\mathbb{X}^T \mathbb{X})^{-1}}{d_{\text{free}}} &= \\ (\mathbb{X}^T \mathbb{X})^{-1} \mathbb{X}^T \sigma_{\varepsilon}^2 \mathbb{1} \mathbb{X} (\mathbb{X}^T \mathbb{X})^{-1} &= \sigma_{\varepsilon}^2 (\mathbb{X}^T \mathbb{X})^{-1}\end{aligned}$$

Where the expected values of the squared residuals are proportional to the diagonal unit matrix $\mathbb{1}$:

$$\frac{\mathbb{E}[\hat{\varepsilon} \hat{\varepsilon}^T]}{d_{\text{free}}} = \sigma_{\varepsilon}^2 \mathbb{1}$$

If any of the predictor matrix columns are close to being *collinear*, then the squared predictor matrix becomes singular, and the covariance of their regression coefficients becomes very large.

The matrix $\mathbb{X}_{\text{inv}} = (\mathbb{X}^T \mathbb{X})^{-1} \mathbb{X}^T$ is the generalized inverse of the *predictor matrix* \mathbb{X} .

```
> # Inverse of predictor matrix squared
> predictor2 <- MASS::ginv(crossprod(predictor))
> # predictor2 <- t(predictor) %*% predictor
> # Variance of residuals
> residvar <- sum(residuals^2)/degf
> # Calculate covariance matrix of betas
> beta_covar <- residvar*predictor2
> # Round(beta_covar, 3)
> betasd <- sqrt(diag(beta_covar))
> all.equal(betasd, modelsum$coeff[, 2], check.attributes=FALSE)
[1] TRUE
> # Calculate t-values of betas
> beta_tvals <- drop(betas)/betasd
> all.equal(beta_tvals, modelsum$coeff[, 3], check.attributes=FALSE)
[1] TRUE
> # Calculate two-sided p-values of betas
> beta_pvals <- 2*pt(-abs(beta_tvals), df=degf)
> all.equal(beta_pvals, modelsum$coeff[, 4], check.attributes=FALSE)
[1] TRUE
> # The square of the generalized inverse is equal
> # to the inverse of the square
> all.equal(MASS::ginv(crossprod(predictor)),
+   invpred %*% t(invpred))
[1] TRUE
```

Covariance Matrix of the Fitted Values

The *fitted values* y_{fit} can also be considered to be *random variables* \hat{y}_{fit} , because the *regression coefficients* $\hat{\beta}$ are *random variables*:

$$\hat{y}_{fit} = \mathbb{X}\hat{\beta} = \mathbb{X}(\beta + \mathbb{X}_{inv}\hat{\epsilon}) = y_{fit} + \mathbb{X}\mathbb{X}_{inv}\hat{\epsilon}.$$

The *covariance matrix* of the *fitted values* σ_{fit}^2 is:

$$\sigma_{fit}^2 = \frac{\mathbb{E}[\mathbb{X}\mathbb{X}_{inv}\hat{\epsilon}(\mathbb{X}\mathbb{X}_{inv}\hat{\epsilon})^T]}{d_{free}} = \frac{\mathbb{E}[\mathbb{H}\hat{\epsilon}\hat{\epsilon}^T\mathbb{H}^T]}{d_{free}} = \frac{\mathbb{H}\mathbb{E}[\hat{\epsilon}\hat{\epsilon}^T]\mathbb{H}^T}{d_{free}} = \sigma_{\epsilon}^2\mathbb{H} = \sigma_{\epsilon}^2\mathbb{X}(\mathbb{X}^T\mathbb{X})^{-1}\mathbb{X}^T$$

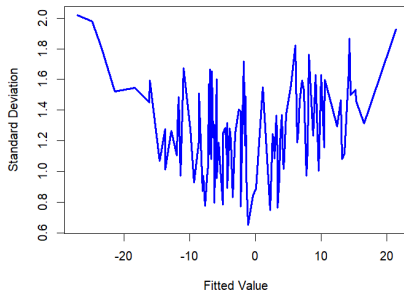
The square of the *influence matrix* \mathbb{H} is equal to itself (it's idempotent): $\mathbb{H}\mathbb{H}^T = \mathbb{H}$.

The variance of the *fitted values* σ_{fit}^2 increases with the distance of the *predictors* from their mean values.

This is because the *fitted values* farther from their mean are more sensitive to the variance of the regression slope.

```
> # Calculate the influence matrix
> influencem <- predictor %%% invpred
> # The influence matrix is idempotent
> all.equal(influencem, influencem %%% influencem)
```

Standard Deviations of Fitted Values
in Multivariate Regression



```
> # Calculate covariance and standard deviations of fitted values
> fitcovar <- residvar*influenem
> fitsd <- sqrt(diag(fitcovar))
> # Sort the standard deviations
> fitsd <- cbind(fitted=fittedv, stddev=fitsd)
> fitsd <- fitsd[order(fittedv), ]
> # Plot the standard deviations
> plot(fitsd, type="l", lwd=3, col="blue",
+      xlab="Fitted Value", ylab="Standard Deviation",
+      main="Standard Deviations of Fitted Values\nin Multivariate Regression")
```

Standard Errors of Time Series Regression

Bootstrapping the regression of asset returns shows that the actual standard errors can be over twice as large as those reported by the function `lm()`.

This is because the function `lm()` assumes that the data is normally distributed, while in reality asset returns have very large skewness and kurtosis.

```
> # Load time series of ETF percentage returns
> retsp <- rutils::etfenv$returns[, c("XLF", "XLE")]
> retsp <- na.omit(retsp)
> nrow <- NROW(retsp)
> head(retsp)
> # Define regression formula
> formulav <- paste(colnames(retsp)[1],
+   paste(colnames(retsp)[-1], collapse="+"),
+   sep=" ~ ")
> # Standard regression
> regmod <- lm(formulav, data=retsp)
> modelsum <- summary(regmod)
> # Bootstrap of regression
> set.seed(1121) # initialize random number generator
> bootd <- sapply(1:100, function(x) {
+   samplev <- sample.int(nrow, replace=TRUE)
+   regmod <- lm(formulav, data=retsp[samplev, ])
+   regmod$coefficients
+ }) # end sapply
> # Means and standard errors from regression
> modelsum$coefficients
> # Means and standard errors from bootstrap
> dim(bootd)
> t(apply(bootd, MARGIN=1,
+   function(x) c(mean=mean(x), stdev=sd(x))))
```

Predictions From *Multivariate Regression Models*

The prediction y_{pred} from a regression model is equal to the *response value* corresponding to the *predictor* vector with the new data \mathbb{X}_{new} :

$$y_{pred} = \mathbb{X}_{new} \beta$$

The prediction is a *random variable* \hat{y}_{pred} , because the *regression coefficients* $\hat{\beta}$ are *random variables*:

$$\hat{y}_{pred} = \mathbb{X}_{new} \hat{\beta} = \mathbb{X}_{new} (\beta + \mathbb{X}_{inv} \hat{\epsilon}) = y_{pred} + \mathbb{X}_{new} \mathbb{X}_{inv} \hat{\epsilon}$$

The variance σ_{pred}^2 of the *predicted value* is:

$$\begin{aligned} \sigma_{pred}^2 &= \frac{\mathbb{E}[\mathbb{X}_{new} \mathbb{X}_{inv} \hat{\epsilon} (\mathbb{X}_{new} \mathbb{X}_{inv} \hat{\epsilon})^T]}{d_{free}} = \\ &= \frac{\mathbb{E}[\mathbb{X}_{new} \mathbb{X}_{inv} \hat{\epsilon} \hat{\epsilon}^T \mathbb{X}_{inv}^T \mathbb{X}_{new}^T]}{d_{free}} = \\ &= \sigma_{\epsilon}^2 \mathbb{X}_{new} \mathbb{X}_{inv} \mathbb{X}_{inv}^T \mathbb{X}_{new}^T = \\ &= \sigma_{\epsilon}^2 \mathbb{X}_{new} (\mathbb{X}^T \mathbb{X})^{-1} \mathbb{X}_{new}^T = \mathbb{X}_{new} \sigma_{\beta}^2 \mathbb{X}_{new}^T \end{aligned}$$

The variance σ_{pred}^2 of the *predicted value* is equal to the *predictor* vector multiplied by the *covariance matrix* of the *regression coefficients* σ_{β}^2 .

```
> # New data predictor is a data frame or row vector
> set.seed(1121)
> newdata <- data.frame(matrix(c(1, rnorm(5)), nr=1))
> colnamev <- colnames(predictor)
> colnames(newdata) <- colnamev
> newdatav <- as.matrix(newdata)
> prediction <- drop(newdatav %*% betas)
> predstd <- drop(sqrt(newdatav %*% beta_covar %*% t(newdatav)))
```

Predictions From *Multivariate Regression* Using `lm()`

The function `predict()` is a *generic function* for forecasting based on a given model.

`predict.lm()` is the predict method for linear models (regressions) produced by the function `lm()`.

In order for `predict.lm()` to work properly, the multivariate regression must be specified using a formula.

```
> # Create formula from text string
> formulav <- paste0("response ~ ",
+   paste(colnames(predictor), collapse=" + "), " - 1")
> # Specify multivariate regression using formula
> regmod <- lm(formulav, data=data.frame(cbind(response, predictor)))
> modelsum <- summary(regmod)
> # Predict from lm object
> predictlm <- predict.lm(object=model, newdata=newdata,
+   interval="confidence", confl=1-2*(1-pnorm(2)))
> # Calculate t-quantile
> tquant <- qt(pnorm(2), df=degf)
> predicthigh <- (prediction + tquant*predsd)
> predictlow <- (prediction - tquant*predsd)
> # Compare with matrix calculations
> all.equal(predictlm[1, "fit"], prediction)
> all.equal(predictlm[1, "lwr"], predictlow)
> all.equal(predictlm[1, "upr"], predicthigh)
```

Total Sum of Squares and Explained Sum of Squares

The *Total Sum of Squares (TSS)* and the *Explained Sum of Squares (ESS)* are defined as:

$$TSS = (y - \bar{y})^T (y - \bar{y})$$

$$ESS = (y_{fit} - \bar{y})^T (y_{fit} - \bar{y})$$

$$RSS = (y - y_{fit})^T (y - y_{fit})$$

Since the *residuals* $\varepsilon = y - y_{fit}$ are orthogonal to the *fitted values* y_{fit} , they are also orthogonal to the *fitted excess values* $(y_{fit} - \bar{y})$:

$$(y - y_{fit})^T (y_{fit} - \bar{y}) = 0$$

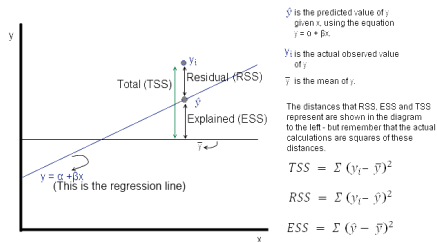
Therefore the *TSS* can be expressed as the sum of the *ESS* plus the *RSS*:

$$TSS = ESS + RSS$$

It also follows that the *RSS* and the *ESS* follow independent *chi-squared* distributions with $(n - k)$ and $(k - 1)$ degrees of freedom.

The degrees of freedom of the *Total Sum of Squares* is equal to the sum of the *RSS* plus the *ESS*:

$$d_{free}^{TSS} = (n - k) + (k - 1) = n - 1.$$



```
> # TSS = ESS + RSS
> tss <- sum((response-mean(response))^2)
> ess <- sum((fittedv-mean(fittedv))^2)
> rss <- sum(residuals^2)
> all.equal(tss, ess + rss)
[1] TRUE
```

R-squared of Multivariate Regression

The *R-squared* is the fraction of the *Explained Sum of Squares (ESS)* divided by the *Total Sum of Squares (TSS)*:

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

The *R-squared* is a measure of the model *goodness of fit*, with *R-squared* close to 1 for models fitting the data very well, and *R-squared* close to 0 for poorly fitting models.

The *R-squared* is equal to the squared correlation between the response and the *fitted values*:

$$\rho_{yyfit} = \frac{(y_{fit} - \bar{y})^T (y - \bar{y})}{\sqrt{TSS \cdot ESS}} = \frac{(y_{fit} - \bar{y})^T (y_{fit} - \bar{y})}{\sqrt{TSS \cdot ESS}} = \sqrt{\frac{ESS}{TSS}}$$

```
> # Set regression attribute for intercept
> attributes(regmod$terms)$intercept <- 1
> # Regression summary
> modelsum <- summary(regmod)
> # Regression R-squared
> rsquared <- ess/tss
> all.equal(rsquared, modelsum$r.squared)
[1] TRUE
> # Correlation between response and fitted values
> cor_fitted <- drop(cor(response, fittedv))
> # Squared correlation between response and fitted values
> all.equal(cor_fitted^2, rsquared)
[1] TRUE
```


Adjusted R-squared of Multivariate Regression

The weakness of *R-squared* is that it increases with the number of predictors (even for predictors which are purely random), so it may provide an inflated measure of the quality of a model with many predictors.

This is remedied by using the *residual variance* ($\sigma_{\varepsilon}^2 = \frac{RSS}{d_{free}}$) instead of the *RSS*, and the *response variance* ($\sigma_y^2 = \frac{TSS}{n-1}$) instead of the *TSS*.

The *adjusted R-squared* is equal to 1 minus the fraction of the *residual variance* divided by the *response variance*:

$$R_{adj}^2 = 1 - \frac{\sigma_{\varepsilon}^2}{\sigma_y^2} = 1 - \frac{RSS/d_{free}}{TSS/(n-1)}$$

Where $d_{free} = (n - k)$ is the number of *degrees of freedom* of the *residuals*.

The *adjusted R-squared* is always smaller than the *R-squared*.

The performance of two different models can be compared by comparing their *adjusted R-squared*, since the model with the larger *adjusted R-squared* has a smaller *residual variance*, so it's better able to explain the *response*.

```
> nrows <- NROW(predictor)
> ncols <- NCOL(predictor)
> # Degrees of freedom of residuals
> degf <- (nrows - ncols)
> # Adjusted R-squared
> rsquared_adj <- (1 - sum(residuals^2)/degf/var(response))
> # Compare adjusted R-squared from lm()
> all.equal(drop(rsquared_adj), modelsum$adj.r.squared)
[1] TRUE
```

Fisher's F -distribution

Let χ_m^2 and χ_n^2 be independent random variables following *chi-squared* distributions with m and n degrees of freedom.

Then the F -statistic random variable:

$$F = \frac{\chi_m^2/m}{\chi_n^2/n}$$

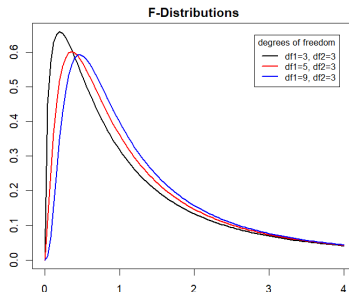
Follows the F -distribution with m and n degrees of freedom, with the probability density function:

$$P(F) = \frac{\Gamma((m+n)/2)m^{m/2}n^{n/2}}{\Gamma(m/2)\Gamma(n/2)} \frac{F^{m/2-1}}{(n+mF)^{(m+n)/2}}$$

The F -distribution depends on the F -statistic F and also on the degrees of freedom, m and n .

The function `df()` calculates the probability density of the F -distribution.

```
> # Plot three curves in loop
> degf <- c(3, 5, 9) # Degrees of freedom
> colorv <- c("black", "red", "blue", "green")
> for (it in 1:NROW(degf)) {
+   curve(expr=df(x, df1=degf[it], df2=3),
+   xlim=c(0, 4), xlab="", ylab="", lwd=2,
+   col=colorv[it], add=as.logical(it-1))
+ } # end for
```



```
> # Add title
> title(main="F-Distributions", line=0.5)
> # Add legend
> labelv <- paste("df", degf, sep="=")
> legend("topright", inset=0.05, title="degrees of freedom",
+       y.intersp=0.5, bty="n", labelv, cex=0.8, lwd=2, lty=1, col=
```

The *F*-test For the Variance Ratio

Let x and y be independent standard *Normal* variables, and let $\sigma_x^2 = \frac{1}{m-1} \sum_{i=1}^m (x_i - \bar{x})^2$ and $\sigma_y^2 = \frac{1}{n-1} \sum_{i=1}^n (y_i - \bar{y})^2$ be their sample variances.

The ratio $F = \sigma_x^2 / \sigma_y^2$ of the sample variances follows the *F*-distribution with m and n degrees of freedom.

The *F*-test tests the *null hypothesis* that the *F*-statistic F is not significantly greater than 1 (the variance σ_x^2 is not significantly greater than σ_y^2).

A large value of the *F*-statistic F indicates that the variances are unlikely to be equal.

The function `pf(q)` returns the cumulative probability of the *F*-distribution, i.e. the cumulative probability that the *F*-statistic F is less than the quantile q .

This *F*-test is very sensitive to the assumption of the normality of the variables.

```
> sigmax <- var(rnorm(nrows))
> sigmay <- var(rnorm(nrows))
> fratio <- sigmax/sigmay
> # Cumulative probability for q = fratio
> pf(fratio, nrows-1, nrows-1)
[1] 0.0642
> # p-value for fratio
> 1-pf((10:20)/10, nrows-1, nrows-1)
[1] 0.500000 0.318150 0.182964 0.096784 0.047876 0.022467 0.010123
[9] 0.001888 0.000793 0.000329
```

The F -statistic for Linear Regression

The performance of two different regression models can be compared by directly comparing their *Residual Sum of Squares* (RSS), since the model with a smaller RSS is better able to explain the *response*.

Let the *restricted* model have p_1 parameters with $df_1 = n - p_1$ degrees of freedom, and the *unrestricted* model have p_2 parameters with $df_2 = n - p_2$ degrees of freedom, with $p_2 < p_1$.

Then the F -statistic F , defined as the ratio of the scaled *Residual Sum of Squares*:

$$F = \frac{(RSS_1 - RSS_2)/(df_1 - df_2)}{RSS_2/df_2}$$

Follows the F -distribution with $(p_2 - p_1)$ and $(n - p_2)$ degrees of freedom (assuming that the *residuals* are normally distributed).

If the *restricted* model only has one parameter (the constant intercept term), then $df_1 = n - 1$, and its *fitted values* are equal to the average of the *response*: $y_i^{fit} = \bar{y}$, so RSS_1 is equal to the TSS :

$RSS_1 = TSS = (y - \bar{y})^2$, so its *Explained Sum of Squares* is equal to zero: $ESS_1 = TSS - RSS_1 = 0$.

Let the *unrestricted* multivariate regression model be defined as:

$$y = \mathbb{X}\beta + \varepsilon$$

Where y is the *response*, \mathbb{X} is the *predictor matrix* (with k *predictors*, including the intercept term), and β are the k *regression coefficients*.

So the *unrestricted* model has k parameters ($p_2 = k$), and $RSS_2 = RSS$ and $ESS_2 = ESS$, and then the F -statistic can be written as:

$$F = \frac{ESS/(k - 1)}{RSS/(n - k)}$$

The F -test for Linear Regression

The *Residual Sum of Squares* $RSS = \varepsilon^T \varepsilon$ and the *Explained Sum of Squares* $ESS = (y_{\text{fit}} - \bar{y})^T (y_{\text{fit}} - \bar{y})$ follow independent *chi-squared* distributions with $(n - k)$ and $(k - 1)$ degrees of freedom.

Then the F -statistic, equal to the ratio of the ESS divided by RSS :

$$F = \frac{ESS/(k - 1)}{RSS/(n - k)}$$

Follows the F -distribution with $(k - 1)$ and $(n - k)$ degrees of freedom (assuming that the *residuals* are normally distributed).

```
> # F-statistic from lm()
> modelsum$fstatistic
value numdf dendif
391      5     94
> # Degrees of freedom of residuals
> degf <- (nrows - ncols)
> # F-statistic from ESS and RSS
> fstat <- (ess/(ncols-1))/(rss/degf)
> all.equal(fstat, modelsum$fstatistic[1], check.attributes=FALSE)
[1] TRUE
> # p-value of F-statistic
> 1-pf(q=fstat, df1=(ncols-1), df2=(nrows-ncols))
[1] 0
```

The Logistic Function

The *logistic* function expresses the probability of a numerical variable ranging over the whole interval of real numbers:

$$p(x) = \frac{1}{1 + \exp(-\lambda x)}$$

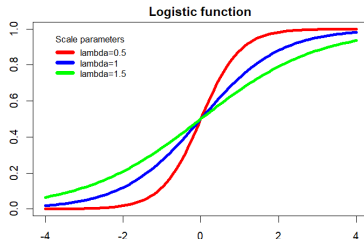
Where λ is the scale (dispersion) parameter.

The *logistic* function is often used as an activation function in neural networks, and logistic regression can be viewed as single neuron network.

The *logistic* function can be inverted to obtain the *Odds Ratio* (the ratio of probabilities for favorable to unfavorable outcomes):

$$\frac{p(x)}{1 - p(x)} = \exp(\lambda x)$$

The function `plogis()` gives the cumulative probability of the *Logistic* distribution,



```
> lambdas <- c(0.5, 1, 1.5)
> colorv <- c("red", "blue", "green")
> # Plot three curves in loop
> for (it in 1:3) {
+   curve(expr=plogis(x, scale=lambdas[it]),
+   xlim=c(-4, 4), type="l", xlab="", ylab="", lwd=4,
+   col=colorv[it], add=(it>1))
+ } # end for
> # Add title
> title(main="Logistic function", line=0.5)
> # Add legend
> legend("topleft", title="Scale parameters",
+   paste("lambda", lambdas, sep=""), y.intersp=0.5,
+   inset=0.05, cex=0.8, lwd=6, bty="n", lty=1, col=colorv)
```

Performing Logistic Regression Using the Function glm()

Logistic regression (*logit*) is used when the response are discrete variables (like factors or integers), when linear regression can't be applied.

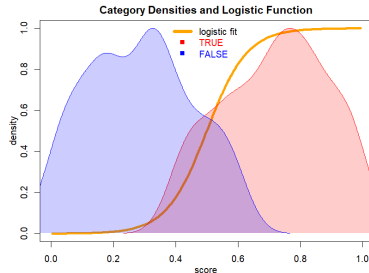
The function `glm()` fits generalized linear models, including logistic regressions.

The parameter `family=binomial(logit)` specifies a binomial distribution of residuals in the logistic regression model.

The *Mann-Whitney test null hypothesis* is that the two samples, x_i and y_i , were obtained from probability distributions with the same median (location).

The function `wilcox.test()` with parameter `paired=FALSE` (the default) calculates the *Mann-Whitney* test statistic and its p -value.

```
> set.seed(1121) # Reset random number generator
> # Simulate overlapping scores data
> sample1 <- runif(100, max=0.6)
> sample2 <- runif(100, min=0.4)
> # Perform Mann-Whitney test for data location
> wilcox.test(sample1, sample2)
> # Combine scores and add categorical variable
> predictor <- c(sample1, sample2)
> response <- c(logical(100), !logical(100))
> # Perform logit regression
> logmod <- glm(response ~ predictor, family=binomial(logit))
> class(logmod)
> summary(logmod)
```



```
> ordern <- order(predictor)
> plot(x=predictor[ordern], y=logmod$fitted.values[ordern],
+      main="Category Densities and Logistic Function",
+      type="l", lwd=4, col="orange", xlab="predictor", ylab="density")
> densityv <- density(predictor[response])
> densityv$y <- densityv$y/max(densityv$y)
> lines(densityv, col="red")
> polygon(c(min(densityv$x), densityv$x, max(densityv$x)), c(min(densityv$y), densityv$y, max(densityv$y)), col="red")
> densityv <- density(predictor[!response])
> densityv$y <- densityv$y/max(densityv$y)
> lines(densityv, col="blue")
> polygon(c(min(densityv$x), densityv$x, max(densityv$x)), c(min(densityv$y), densityv$y, max(densityv$y)), col="blue")
> # Add legend
> legend(x="top", cex=1.0, bty="n", lty=c(1, NA, NA),
+       lwd=c(6, NA, NA), pch=c(NA, 15, 15), bty="n", y.intersp=0.5,
+       legend=c("logistic fit", "TRUE", "FALSE"),
+       col=c("orange", "red", "blue"),
+       text.col=c("black", "red", "blue"))
```

The Likelihood Function of the Binomial Distribution

Let b be a binomial random variable, which either has the value $b = 1$ with probability p , or $b = 0$ with probability $(1 - p)$.

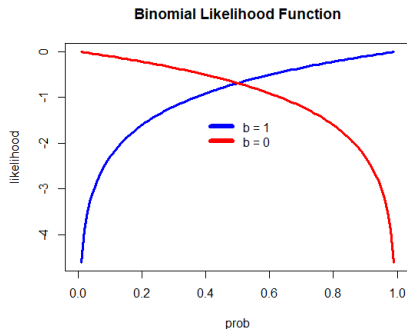
Then b follows the binomial distribution:

$$f(b) = b p + (1 - b) (1 - p)$$

The *log-likelihood* function $\mathcal{L}(p|b)$ of the probability p given the value b is obtained from the logarithms of the binomial probabilities:

$$\mathcal{L}(p|b) = b \log(p) + (1 - b) \log(1 - p)$$

The *log-likelihood* function measures how *likely* are the distribution parameters, given the observed values.



```
> # Likelihood function of binomial distribution
> likefun <- function(prob, b) {
+   b*log(prob) + (1-b)*log(1-prob)
+ } # end likefun
> likefun(prob=0.25, b=1)
> # Plot binomial likelihood function
> curve(expr=likefun(x, b=1), xlim=c(0, 1), lwd=3,
+       xlab="prob", ylab="likelihood", col="blue",
+       main="Binomial Likelihood Function")
> curve(expr=likefun(x, b=0), lwd=3, col="red", add=TRUE)
> legend(x="top", legend=c("b = 1", "b = 0"),
+       title=NULL, inset=0.3, cex=1.0, lwd=6, y.intersp=0.5,
+       bty="n", lty=1, col=c("blue", "red"))
```


The Likelihood Function of the Logistic Model

Let b_i be binomial random variables, with probabilities p_i that depend on the numerical variables s_i through the logistic function:

$$p_i = \frac{1}{1 + \exp(-\lambda_0 - \lambda_1 s_i)}$$

Let's assume that the b_i and s_i values are known (observed), and we want to find the parameters λ_0 and λ_1 that best fit the observations.

The *log-likelihood* function \mathcal{L} is equal to the sum of the individual *log-likelihoods*:

$$\mathcal{L}(\lambda_0, \lambda_1 | b_i) = \sum_{i=1}^n b_i \log(p_i) + (1 - b_i) \log(1 - p_i)$$

The *log-likelihood* function measures how *likely* are the distribution parameters, given the observed values.

```
> # Specify predictor matrix
> predictor=cbind(intercept=rep(1, NROW(response)), predictor)
> # Likelihood function of the logistic model
> likefun <- function(coeff, response, predictor) {
+   probs <- plogis(drop(predictor %*% coeff))
+   -sum(response*log(probs) + (1-response)*log((1-probs)))
+ } # end likefun
> # Run likelihood function
> coeff <- c(1, 1)
> likefun(coeff, response, predictor)
```

Multi-dimensional Optimization Using optim()

The function `optim()` performs *multi-dimensional* optimization.

The argument `fn` is the objective function to be minimized.

The argument of `fn` that is to be optimized, must be a vector argument.

The argument `par` is the initial vector argument value.

`optim()` accepts additional parameters bound to the dots `"..."` argument, and passes them to the `fn` objective function.

The arguments `lower` and `upper` specify the search range for the variables of the objective function `fn`.

`method="L-BFGS-B"` specifies the quasi-Newton *gradient* optimization method.

`optim()` returns a list containing the location of the minimum and the objective function value.

The *gradient* methods used by `optim()` can only find the local minimum, not the global minimum.

```
> # Rastrigin function with vector argument for optimization
> rastrigin <- function(vectorv, param=25) {
+   sum(vectorv^2 - param*cos(vectorv))
+ } # end rastrigin
> vectorv <- c(pi/6, pi/6)
> rastrigin(vectorv=vectorv)
> # Draw 3d surface plot of Rastrigin function
> options(rgl.useNULL=TRUE); library(rgl)
> rgl::persp3d(
+   x=Vectorize(function(x, y) rastrigin(vectorv=c(x, y))),
+   xlim=c(-10, 10), ylim=c(-10, 10),
+   col="green", axes=FALSE, zlab="", main="rastrigin")
> # Render the 3d surface plot of function
> rgl::rglwidget(elementId="plot3drgl", width=400, height=400)
> # Optimize with respect to vector argument
> optim1 <- optim(par=vectorv, fn=rastrigin,
+   method="L-BFGS-B",
+   upper=c(4*pi, 4*pi),
+   lower=c(pi/2, pi/2),
+   param=1)
> # Optimal parameters and value
> optim1$par
> optim1$value
> rastrigin(optim1$par, param=1)
```

Maximum Likelihood Calibration of the Logistic Model

The logistic model depends on the unknown parameters λ_0 and λ_1 , which can be calibrated by maximizing the likelihood function.

The function `optim()` with the argument `hessian=TRUE` returns the Hessian matrix.

The Hessian is a matrix of the second-order partial derivatives of the likelihood function with respect to the optimization parameters:

$$H = \frac{\partial^2 \mathcal{L}}{\partial \lambda^2}$$

The Hessian matrix measures the convexity of the likelihood surface - it's large if the likelihood surface is highly convex, and it's small if the likelihood surface is flat.

If the likelihood surface is highly convex, then the coefficients can be determined with greater precision, so their standard errors are small. If the likelihood surface is flat, then the coefficients have large standard errors.

The inverse of the Hessian matrix provides the standard errors of the logistic parameters: $\sigma_{SE} = \sqrt{H^{-1}}$.

```
> # Initial parameters
> initp <- c(1, 1)
> # Find max likelihood parameters using steepest descent optimizer
> optim1 <- optim(par=initp,
+               fn=likefun, # Log-likelihood function
+               method="L-BFGS-B", # Quasi-Newton method
+               response=response,
+               predictor=predictor,
+               upper=c(20, 20), # Upper constraint
+               lower=c(-20, -20), # Lower constraint
+               hessian=TRUE)
> # Optimal logistic parameters
> optim1$par
> unname(logmod$coefficients)
> # Standard errors of parameters
> sqrt(diag(solve(optim1$hessian)))
> modelsum <- summary(logmod)
> modelsum$coefficients[, 2]
```

Package *ISLR* With Datasets for Machine Learning

The package *ISLR* contains datasets used in the book *Introduction to Statistical Learning* by Gareth James, Daniela Witten, Trevor Hastie, and Robert Tibshirani.

The book introduces machine learning techniques using R, and it's a must for advanced finance applications.

```
> library(ISLR) # Load package ISLR
> # get documentation for package tseries
> packageDescription("ISLR") # get short description
>
> help(package="ISLR") # Load help page
>
> library(ISLR) # Load package ISLR
>
> data(package="ISLR") # list all datasets in ISLR
>
> ls("package:ISLR") # list all objects in ISLR
>
> detach("package:ISLR") # Remove ISLR from search path
```

The Default Dataset

The data frame `Default` in the package *ISLR* contains credit default data.

The `Default` data frame contains two columns of categorical data (factors): `default` and `student`, and two columns of numerical data: `balance` and `income`.

The columns `default` and `student` contain factor data, and they can be converted to Boolean values, with `TRUE` if `default == "Yes"` and `student == "Yes"`, and `FALSE` otherwise.

This avoids implicit coercion by the function `glm()`.

```
> # Coerce the student and default columns into Boolean
> Default <- ISLR::Default
> Default$default <- (Default$default == "Yes")
> Default$student <- (Default$student == "Yes")
> colnames(Default)[1:2] <- c("default", "student")
> attach(Default) # Attach Default to search path
> # Explore credit default data
> summary(Default)
```

default	student	balance	income
Mode :logical	Mode :logical	Min. : 0	Min. : 772
FALSE:9667	FALSE:7056	1st Qu.: 482	1st Qu.:21340
TRUE :333	TRUE :2944	Median : 824	Median :34553
		Mean : 835	Mean :33517
		3rd Qu.:1166	3rd Qu.:43808
		Max. :2654	Max. :73554

```
> sapply(Default, class)
  default student balance income
"logical" "logical" "numeric" "numeric"
> dim(Default)
[1] 10000    4
> head(Default)
```

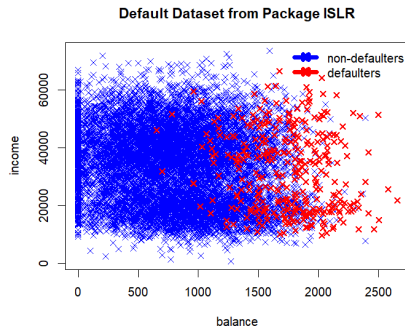
	default	student	balance	income
1	FALSE	FALSE	730	44362
2	FALSE	TRUE	817	12106
3	FALSE	FALSE	1074	31767
4	FALSE	FALSE	529	35704
5	FALSE	FALSE	786	38463
6	FALSE	TRUE	920	7492

The Dependence of default on The balance and income

The columns student, balance, and income can be used as *predictors* to predict the default column.

The scatterplot of income versus balance shows that the balance column is able to separate the data points of default = TRUE from default = FALSE.

But there is very little difference in income between the default = TRUE versus default = FALSE data points.



```
> # Plot data points for non-defaulters
> xlim <- range(balance); ylim <- range(income)
> plot(income ~ balance,
+       main="Default Dataset from Package ISLR",
+       xlim=xlim, ylim=ylim, pch=4, col="blue",
+       data=Default[!default, ])
> # Plot data points for defaulters
> points(income ~ balance, pch=4, lwd=2, col="red",
+        data=Default[default, ])
> # Add legend
> legend(x="topright", legend=c("non-defaulters", "defaulters"),
+        y.intersp=0.5, bty="n", col=c("blue", "red"), lty=1, lwd=6, pch=4)
```

Boxplots of the Default Dataset

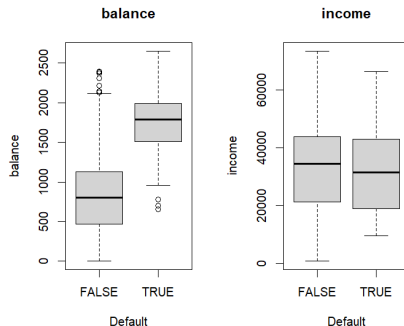
A *Box Plot* (box-and-whisker plot) is a graphical display of a distribution of data:

The *box* represents the upper and lower quartiles, The vertical lines (whiskers) represent values beyond the quartiles, Open circles represent values beyond the nominal range (outliers).

The function `boxplot()` plots a box-and-whisker plot for a distribution of data.

`boxplot()` has two methods: one for formula objects (involving categorical variables), and another for data frames.

The *Mann-Whitney* test shows that the *balance* column provides a strong separation between defaulters and non-defaulters, but the *income* column doesn't.



```
> # Perform Mann-Whitney test for the location of the balances
> wilcox.test(balance[default], balance[!default])
> # Perform Mann-Whitney test for the location of the incomes
> wilcox.test(income[default], income[!default])
```

```
> x11(width=6, height=5)
> # Set 2 plot panels
> par(mfrow=c(1,2))
> # Balance boxplot
> boxplot(formula=balance ~ default,
+   col="lightgrey", main="balance", xlab="Default")
> # Income boxplot
> boxplot(formula=income ~ default,
+   col="lightgrey", main="income", xlab="Default")
```

Modeling Credit Defaults Using *Logistic Regression*

The balance column can be used to calculate the probability of default using *logistic regression*.

The residuals are the differences between the actual response values (0 and 1), and the calculated probabilities of default.

The residuals are not normally distributed, so the data is fitted using the *maximum likelihood* method, instead of least squares.

```
> # Fit logistic regression model
> logmod <- glm(default ~ balance, family=binomial(logit))
> class(logmod)
[1] "glm" "lm"
> summary(logmod)
```

```
Call:
glm(formula = default ~ balance, family = binomial(logit))
```

Deviance Residuals:

Min	1Q	Median	3Q	Max
-2.270	-0.146	-0.059	-0.022	3.759

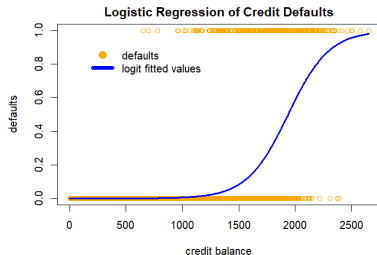
Coefficients:

	Estimate	Std. Error	z value	Pr(> z)
(Intercept)	-10.65133	0.36116	-29.5	<2e-16 ***
balance	0.00550	0.00022	24.9	<2e-16 ***

```
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

```
(Dispersion parameter for binomial family taken to be 1)
```

```
Null deviance: 2920.6  on 9999  degrees of freedom
Residual deviance: 1596.5  on 9998  degrees of freedom
AIC: 1600
```



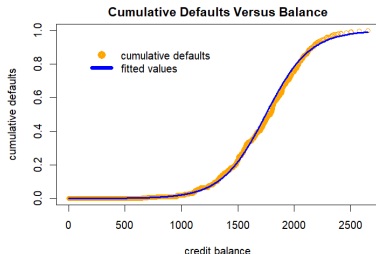
```
> x11(width=6, height=5)
> par(mar=c(4, 4, 2, 2), oma=c(0, 0, 0, 0), mgp=c(2.5, 1, 0))
> plot(x=balance, y=default,
+      main="Logistic Regression of Credit Defaults",
+      col="orange", xlab="credit balance", ylab="defaults")
> ordern <- order(balance)
> lines(x=balance[ordern], y=logmod$fitted.values[ordern], col="blue")
> legend(x="topleft", inset=0.1, bty="n", lwd=6, y.intersp=0.5,
+      legend=c("defaults", "logit fitted values"),
+      col=c("orange", "blue"), lty=c(NA, 1), pch=c(1, NA))
```


Modeling Cumulative Defaults Using *Logistic Regression*

The function `glm()` can model a *logistic* regression using either a Boolean response variable, or using a response variable specified as a frequency.

In the second case, the response variable should be defined as a two-column matrix, with the cumulative frequency of success (TRUE) and a cumulative frequency of failure (FALSE).

These two different ways of specifying the *logistic* regression are related, but they are not equivalent, because they have different error terms.



```
> # Calculate cumulative defaults
> sumd <- sum(default)
> defaultv <- sapply(balance, function(lim) {
+   sum(default[balance <= lim])
+ }) # end sapply
> # Perform logit regression
> logmod <- glm(cbind(defaultv, sumd-defaultv) ~ balance,
+   family=binomial(logit))
> summary(logmod)
```

```
> plot(x=balance, y=defaultv/sumd, col="orange", lwd=1,
+   main="Cumulative Defaults Versus Balance",
+   xlab="credit balance", ylab="cumulative defaults")
> ordern <- order(balance)
> lines(x=balance[ordern], y=logmod$fitted.values[ordern],
+   col="blue", lwd=3)
> legend(x="topleft", inset=0.1, bty="n", y.intersp=0.5,
+   legend=c("cumulative defaults", "fitted values"),
+   col=c("orange", "blue"), lty=c(NA, 1), pch=c(1, NA), lwd=6)
```

Multifactor Logistic Regression

Logistic regression calculates the probability of categorical variables, from the *Odds Ratio* of continuous predictors:

$$p = \frac{1}{1 + \exp(-\lambda_0 - \sum_{i=1}^n \lambda_i x_i)}$$

The *generic* function `summary()` produces a list of regression model summary and diagnostic statistics:

- coefficients: matrix with estimated coefficients, their z-values, and p-values,
- *Null* deviance: measures the differences between the response values and the probabilities calculated using only the intercept,
- *Residual* deviance: measures the differences between the response values and the model probabilities,

The *balance* and *student* columns are statistically significant, but the *income* column is not.

```
> # Fit multifactor logistic regression model
> colnamev <- colnames(Default)
> formulav <- as.formula(paste(colnamev[1],
+   paste(colnamev[-1], collapse="+"), sep=" ~ "))
> formulav
default ~ student + balance + income
> logmod <- glm(formulav, data=Default, family=binomial(logit))
> summary(logmod)
```

Call:
glm(formula = formulav, family = binomial(logit), data = Default)

Deviance Residuals:

Min	1Q	Median	3Q	Max
-2.469	-0.142	-0.056	-0.020	3.738

Coefficients:

	Estimate	Std. Error	z value	Pr(> z)
(Intercept)	-1.09e+01	4.92e-01	-22.08	<2e-16 ***
studentTRUE	-6.47e-01	2.36e-01	-2.74	0.0062 **
balance	5.74e-03	2.32e-04	24.74	<2e-16 ***
income	3.03e-06	8.20e-06	0.37	0.7115

Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

(Dispersion parameter for binomial family taken to be 1)

Null deviance: 2920.6 on 9999 degrees of freedom
Residual deviance: 1571.5 on 9996 degrees of freedom
AIC: 1580

Number of Fisher Scoring iterations: 8

Confounding Variables in Multifactor Logistic Regression

The student column alone can be used to calculate the probability of default using single-factor *logistic* regression.

But the coefficient from the single-factor regression is positive (indicating that students are more likely to default), while the coefficient from the multifactor regression is negative (indicating that students are less likely to default).

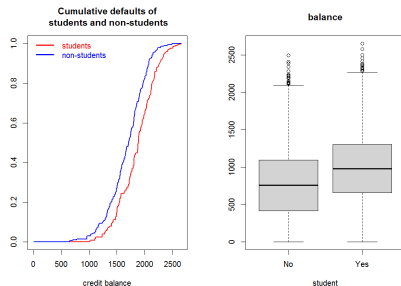
The reason that students are more likely to default is because they have higher credit balances than non-students - which is what the single-factor regression shows.

But students are less likely to default than non-students that have the same credit balance - which is what the multifactor model shows.

The student column is a confounding variable since it's correlated with the balance column.

That's why the multifactor regression coefficient for student is negative, while the single factor coefficient for student is positive.

```
> # Fit single-factor logistic model with student as predictor
> glm_student <- glm(default ~ student, family=binomial(logit))
> summary(glm_student)
> # Multifactor coefficient is negative
> logmod$coefficients
> # Single-factor coefficient is positive
> glm_student$coefficients
```



```
> # Calculate cumulative defaults
> cum_defaults <- sapply(balance, function(lim) {
+   c(student=sum(default[student & (balance <= lim)]),
+     non_student=sum(default[!student & (balance <= lim)]))
+ }) # end sapply
> total_defaults <- c(student=sum(student & default),
+   student=sum(!student & default))
> cum_defaults <- t(cum_defaults / total_defaults)
> # Plot cumulative defaults
> par(mfrow=c(1,2)) # Set plot panels
> ordern <- order(balance)
> plot(x=balance[ordern], y=cum_defaults[ordern, 1],
+   col="red", t="l", lwd=2, xlab="credit balance", ylab="",
+   main="Cumulative defaults of\n students and non-students")
> lines(x=balance[ordern], y=cum_defaults[ordern, 2], col="blue", lwd=2)
> legend(x="topleft", bty="n", y.intersp=0.5,
+   legend=c("students", "non-students"),
+   col=c("red", "blue"), text.col=c("red", "blue"), lwd=3)
> # Balance boxplot for student factor
```

Forecasting Credit Defaults using Logistic Regression

The function `predict()` is a *generic function* for forecasting based on a given model.

The method `predict.glm()` produces forecasts for a generalized linear (*glm*) model, in the form of numeric probabilities, not the Boolean response variable.

The Boolean forecasts are obtained by comparing the *forecast probabilities* with a *discrimination threshold*.

Let the *null hypothesis* be that the subject will not default: `default = FALSE`.

If the *forecast probability* is *less* than the *discrimination threshold*, then the forecast is that the subject will not default and that the *null hypothesis* is TRUE.

The *in-sample forecasts* are just the *fitted values* of the *glm* model.

```
> # Perform in-sample forecast from logistic regression model
> forecastv <- predict(logmod, type="response")
> all.equal(logmod$fitted.values, forecastv)
[1] TRUE
> # Define discrimination threshold value
> threshold <- 0.7
> # Calculate confusion matrix in-sample
> table(actual=!default, forecast=(forecastv < threshold))
      forecast
actual FALSE TRUE
  FALSE   57  276
   TRUE   12 9655
> # Fit logistic regression over training data
> set.seed(1121) # Reset random number generator
> nrows <- NROW(Default)
> samplev <- sample.int(n=nrows, size=nrows/2)
> traindata <- Default[samplev, ]
> logmod <- glm(formulav, data=traindata, family=binomial(logit))
> # Forecast over test data out-of-sample
> testdata <- Default[~samplev, ]
> forecastv <- predict(logmod, newdata=testdata, type="response")
> # Calculate confusion matrix out-of-sample
> table(actual=!testdata$default, forecast=(forecastv < threshold))
      forecast
actual FALSE TRUE
  FALSE   29  132
   TRUE    9 4830
```

Forecasting Errors

A *binary classification model* categorizes cases based on its forecasts whether the *null hypothesis* is TRUE or FALSE.

Let the *null hypothesis* be that the subject will not default: `default = FALSE`.

A *positive* result corresponds to rejecting the null hypothesis, while a *negative* result corresponds to accepting the null hypothesis.

The forecasts are subject to two different types of errors: *type I* and *type II* errors.

A *type I* error is the incorrect rejection of a TRUE *null hypothesis* (i.e. a "false positive"), when there is no default but it's classified as a default.

A *type II* error is the incorrect acceptance of a FALSE *null hypothesis* (i.e. a "false negative"), when there is a default but it's classified as no default.

```
> # Calculate confusion matrix out-of-sample
> confmat <- table(actual=!testdata$default,
+ forecast=(forecastv < threshold))
> confmat
      forecast
actual FALSE TRUE
FALSE    29  132
TRUE     9 4830
> # Calculate FALSE positive (type I error)
> sum(!testdata$default & (forecastv > threshold))
[1] 9
> # Calculate FALSE negative (type II error)
> sum(testdata$default & (forecastv < threshold))
[1] 132
```

The Confusion Matrix of a Binary Classification Model

The confusion matrix summarizes the performance of a classification model on a set of test data for which the actual values of the *null hypothesis* are known.

		Forecast	
		Null is FALSE	Null is TRUE
Actual	Null is FALSE	True Positive (sensitivity)	False Negative (type II error)
	Null is TRUE	False Positive (type I error)	True Negative (specificity)

```
> # Calculate FALSE positive and FALSE negative rates
> confmat <- confmat / rowSums(confmat)
> c(typeI=confmat[2, 1], typeII=confmat[1, 2])
typeI typeII
0.00186 0.81988
> detach(Default)
```

Let the *null hypothesis* be that the subject will not default: default = FALSE.

The *true positive rate* (known as the *sensitivity*) is the fraction of FALSE *null hypothesis* cases that are correctly classified as FALSE.

The *false negative rate* is the fraction of FALSE *null hypothesis* cases that are incorrectly classified as TRUE (*type II error*).

The sum of the *true positive* plus the *false negative* rate is equal to 1.

The *true negative rate* (known as the *specificity*) is the fraction of TRUE *null hypothesis* cases that are correctly classified as TRUE.

The *false positive rate* is the fraction of TRUE *null hypothesis* cases that are incorrectly classified as FALSE (*type I error*).

The sum of the *true negative* plus the *false positive* rate is equal to 1.

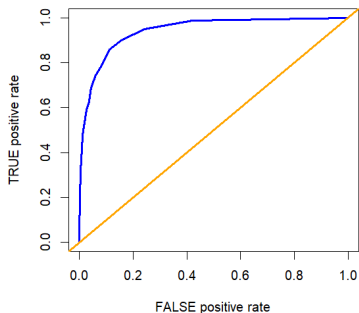
Receiver Operating Characteristic (ROC) Curve

The *ROC curve* is the plot of the *true positive rate*, as a function of the *false positive rate*, and illustrates the performance of a binary classifier.

The area under the *ROC curve* (AUC) is a measure of the performance of a binary classification model.

```
> # Confusion matrix as function of threshold
> confun <- function(actualv, forecastv, threshold) {
+   confmat <- table(actualv, (forecastv < threshold))
+   confmat <- confmat / rowSums(confmat)
+   c(typeI=confmat[2, 1], typeII=confmat[1, 2])
+ } # end confun
> confun(!testdata$default, forecastv, threshold=threshold)
> # Define vector of discrimination thresholds
> threshv <- seq(0.05, 0.95, by=0.05)^2
> # Calculate error rates
> error_rates <- sapply(threshv, confun,
+   actualv=!testdata$default, forecastv=forecastv) # end sapply
> error_rates <- t(error_rates)
> rownames(error_rates) <- threshv
> error_rates <- rbind(c(1, 0), error_rates)
> error_rates <- rbind(error_rates, c(0, 1))
> # Calculate area under ROC curve (AUC)
> truepos <- (1 - error_rates[, "typeII"])
> truepos <- (truepos + rutils::lagit(truepos))/2
> falsepos <- rutils::diffit(error_rates[, "typeI"])
> abs(sum(truepos*falsepos))
```

ROC Curve for Defaults



```
> # Plot ROC Curve for Defaults
> x11(width=5, height=5)
> plot(x=error_rates[, "typeI"], y=1-error_rates[, "typeII"],
+   xlab="FALSE positive rate", ylab="TRUE positive rate",
+   main="ROC Curve for Defaults", type="l", lwd=3, col="blue")
> abline(a=0.0, b=1.0, lwd=3, col="orange")
```

Reading TAQ Data From .csv Files

Trade and Quote (TAQ) data stored in .csv files can be very large, so it's better to read it using the function `data.table::fread()` which is much faster than the function `read.csv()`.

Each *trade* or *quote* contributes a *tick* (row) of data, and the number of ticks can be very large (hundred of thousands per day, or more).

The function `strptime()` coerces character strings representing the date and time into POSIXlt *date-time* objects.

The argument `format="%H:%M:%OS"` allows the parsing of fractional seconds, for example "15:59:59.989847074".

The function `as.POSIXct()` coerces objects into POSIXct *date-time* objects, with a numeric value representing the *moment of time* in seconds.

```
> library(HighFreq)
> # Read TAQ trade data from csv file
> taq <- data.table::fread(file="/Users/jerzy/Develop/data/xxl_tick
> # Inspect the TAQ data
> taq
> class(taq)
> colnames(taq)
> sapply(taq, class)
> symbol <- taq$SYM_ROOT[1]
> # Create date-time index
> dates <- paste(taq$DATE, taq$TIME_M)
> # Coerce date-time index to POSIXlt
> dates <- strptime(dates, "%Y%m%d %H:%M:%OS")
> class(dates)
> # Display more significant digits
> # options("digits")
> options(digits=20, digits.secs=10)
> last(dates)
> unclass(last(dates))
> as.numeric(last(dates))
> # Coerce date-time index to POSIXct
> dates <- as.POSIXct(dates)
> class(dates)
> last(dates)
> unclass(last(dates))
> as.numeric(last(dates))
> # Calculate the number of ticks per second
> nsecs <- as.numeric(last(dates)) - as.numeric(first(dates))
> NROW(taq)/(6.5*3600)
> # Select TAQ data columns
> taq <- taq[, .(price=PRICE, volume=SIZE)]
> # Add date-time index
> taq <- cbind(index=dates, taq)
```


Microstructure Noise in High Frequency Data

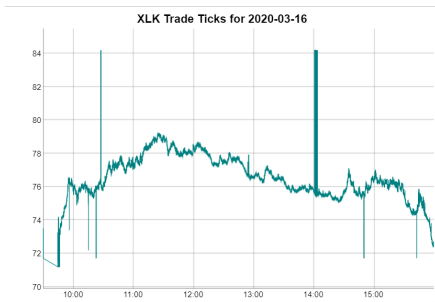
High frequency data contains *microstructure noise* in the form of *price jumps* and the *bid-ask bounce*.

Price jumps are single ticks with prices far away from the average.

Price jumps are often caused by data collection errors, but sometimes they represent actual very large lot trades.

The *bid-ask bounce* is the bouncing of traded prices between the bid and ask prices.

The *bid-ask bounce* creates an illusion of rapidly changing prices, while in fact the mid price is constant.



```
> # Coerce trade ticks to xts series
> xtsv <- xts::xts(taq[, .(price, volume)], taq$index)
> colnames(xtsv) <- paste(symbol, c("Close", "Volume"), sep=".")
> save(xtsv, file="/Users/jerzy/Develop/data/xlk_tick_trades2020_0316.Rsave")
> # save(xtsv, file="/Users/jerzy/Develop/data/xlk_tick_trades2020_0316.Rsave")
> # Plot dygraph
> dygraphs::dygraph(xtsv$XLK.Close,
+   main="XLK Trade Ticks for 2020-03-16")
> # Plot in x11 window
> x11(width=6, height=5)
> quantmod::chart_Series(x=xtsv$XLK.Close,
+   name="XLK Trade Ticks for 2020-03-16")
```

Removing Microstructure Noise From High Frequency Data

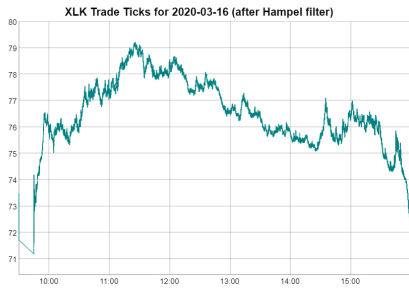
Microstructure noise can be removed from high frequency data by using a *Hampel filter*.

The *z-scores* are equal to the prices minus the median prices, divided by the median absolute deviation (*MAD*) of prices:

$$z_i = \frac{p_i - \text{median}(p)}{\text{MAD}}$$

If the *z-score* exceeds the *threshold value* then it's classified as an *outlier* (jump in prices).

```
> # Calculate centered Hampel filter to remove price jumps
> look_back <- 111
> half_back <- look_back %/% 2
> medianv <- roll::roll_median(taq$price, width=look_back)
> # medianv <- TTR::runMedian(taq$price, n=look_back)
> medianv <- rutils::lagit(medianv, lagg=(-half_back), pad_zeros=F)
> madv <- HighFreq::roll_var(matrix(taq$price), look_back=look_back)
> # madv <- TTR::runMAD(taq$price, n=look_back)
> madv <- rutils::lagit(madv, lagg=(-half_back), pad_zeros=FALSE)
> # Calculate Z-scores
> zscores <- (taq$price - medianv)/madv
> zscores[is.na(zscores)] <- 0
> zscores[!is.finite(zscores)] <- 0
> sum(is.na(zscores))
> sum(!is.finite(zscores))
> range(zscores); mad(zscores)
> hist(zscores, breaks=2000, xlim=c(-5*mad(zscores), 5*mad(zscores))
```



```
> # Define discrimination threshold value
> threshold <- 6*mad(zscores)
> # Remove price jumps with large z-scores
> bad_ticks <- (abs(zscores) > threshold)
> good_ticks <- taq[!bad_ticks]
> # Calculate number of price jumps
> sum(bad_ticks)/NROW(zscores)
> # Coerce trade prices to xts
> xtsv <- xts::xts(good_ticks[, .(price, volume)], good_ticks$index)
> colnames(xtsv) <- c("XLK.Close", "XLK.Volume")
> # Plot dygraph of the clean lots
> dygraphs::dygraph(xtsv$XLK.Close,
+   main="XLK Trade Ticks for 2020-03-16 (Hampel filtered)")
> # Plot the large lots
> x11(width=6, height=5)
> quantmod::chart_Series(x=xtsv$XLK.Close,
+   name="XLK Trade Ticks for 2020-03-16 (Hampel filtered)")
```

Classifying Data Outliers Using the Hampel Filter

The data points whose absolute *z-scores* exceed a *threshold value* are classified as outliers.

This procedure is a *classifier*, which classifies the prices as either good or bad data points.

If the bad data points are not labeled, then we can add jumps to the data to test the performance of the classifier.

Let the *null hypothesis* be that the given price is a good data point.

A positive result corresponds to rejecting the *null hypothesis*, while a negative result corresponds to accepting the *null hypothesis*.

The classifications are subject to two different types of errors: *type I* and *type II* errors.

A *type I* error is the incorrect rejection of a TRUE *null hypothesis* (i.e. a "false positive"), when good data is classified as bad.

A *type II* error is the incorrect acceptance of a FALSE *null hypothesis* (i.e. a "false negative"), when bad data is classified as good.

```
> # Define discrimination threshold value
> threshold <- 6*mad(zscores)
> # Calculate number of prices classified as bad data
> isbad <- (abs(zscores) > threshold)
> sum(isbad)
> # Add 200 random price jumps into prices
> set.seed(1121)
> nbad <- 200
> isjump <- logical(NROW(closep))
> isjump[sample(x=NROW(isjump), size=nbad)] <- TRUE
> closep[isjump] <- closep[isjump]*
+   sample(c(0.95, 1.05), size=nbad, replace=TRUE)
> # Plot prices and medians
> dygraphs::dygraph(cbind(closep, medianv), main="VTI median") %>%
+   dyOptions(colors=c("black", "red"))
> # Calculate time series of z-scores
> medianv <- roll::roll_median(closep, width=look_back)
> # medianv <- TTR::runMedian(closep, n=look_back)
> madv <- HighFreq::roll_var(closep, look_back=look_back, method="n")
> # madv <- TTR::runMAD(closep, n=look_back)
> zscores <- (closep - medianv)/madv
> zscores[1:look_back, ] <- 0
> # Calculate number of prices classified as bad data
> isbad <- (abs(zscores) > threshold)
> sum(isbad)
```

Confusion Matrix of a Binary Classification Model

A *binary classification model* categorizes cases based on its forecasts whether the *null hypothesis* is TRUE or FALSE.

The confusion matrix summarizes the performance of a classification model on a set of test data for which the actual values of the *null hypothesis* are known.

		Forecast	
		Null is FALSE	Null is TRUE
Actual	Null is FALSE	True Positive (sensitivity)	False Negative (type II error)
	Null is TRUE	False Positive (type I error)	True Negative (specificity)

```
> # Calculate confusion matrix
> table(actual=!isjump, forecast=!isbad)
> sum(isbad)
> # FALSE positive (type I error)
> sum(!isjump & isbad)
> # FALSE negative (type II error)
> sum(isjump & !isbad)
```

Let the *null hypothesis* be that the given price is a good data point.

The *true positive rate* (known as the *sensitivity*) is the fraction of FALSE *null hypothesis* cases that are correctly classified as FALSE.

The *false negative rate* is the fraction of FALSE *null hypothesis* cases that are incorrectly classified as TRUE (*type II error*).

The sum of the *true positive* plus the *false negative* rate is equal to 1.

The *true negative rate* (known as the *specificity*) is the fraction of TRUE *null hypothesis* cases that are correctly classified as TRUE.

The *false positive rate* is the fraction of TRUE *null hypothesis* cases that are incorrectly classified as FALSE (*type I error*).

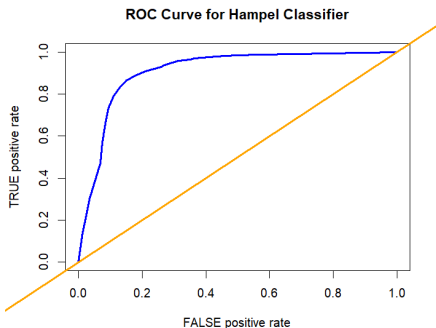
The sum of the *true negative* plus the *false positive* rate is equal to 1.

Receiver Operating Characteristic (ROC) Curve

The *ROC curve* is the plot of the *true positive rate*, as a function of the *false positive rate*, and illustrates the performance of a binary classifier.

The area under the *ROC curve* (AUC) measures the classification ability of a binary classifier.

```
> # Confusion matrix as function of threshold
> confun <- function(actualv, zscores, threshold) {
+   confmat <- table(!actualv, !(abs(zscores) > threshold))
+   confmat <- confmat / rowSums(confmat)
+   c(typeI=confmat[2, 1], typeII=confmat[1, 2])
+ } # end confun
> confun(isjump, zscores, threshold=threshold)
> # Define vector of discrimination thresholds
> threshv <- seq(from=0.2, to=5.0, by=0.2)
> # Calculate error rates
> error_rates <- sapply(threshv, confun,
+   actualv=isjump, zscores=zscores) # end sapply
> error_rates <- t(error_rates)
> rownames(error_rates) <- threshv
> error_rates <- rbind(c(1, 0), error_rates)
> error_rates <- rbind(error_rates, c(0, 1))
> # Calculate area under ROC curve (AUC)
> truepos <- (1 - error_rates[, "typeII"])
> truepos <- (truepos + rutils::lagit(truepos))/2
> falsepos <- rutils::diffit(error_rates[, "typeI"])
> abs(sum(truepos*falsepos))
```



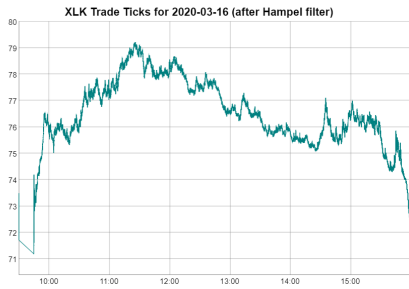
```
> # Plot ROC curve for Hampel classifier
> x11(width=6, height=5)
> plot(x=error_rates[, "typeI"], y=1-error_rates[, "typeII"],
+   xlab="FALSE positive rate", ylab="TRUE positive rate",
+   xlim=c(0, 1), ylim=c(0, 1),
+   main="ROC Curve for Hampel Classifier",
+   type="l", lwd=3, col="blue")
> abline(a=0.0, b=1.0, lwd=3, col="orange")
```

Improved Microstructure Noise Filtering

The filtering of microstructure noise can be improved by calculating the median prices over an interval of only 3 data points.

If the *z-score* exceeds the *threshold value* then it's classified as an *outlier* (jump in prices).

```
> # Calculate centered Hampel filter over 3 data points
> medianv <- roll::roll_median(taq$price, width=3)
> medianv[1:2] <- taq$price[1:2]
> medianv <- rutils::lagit(medianv, lagg=-1, pad_zeros=FALSE)
> madv <- HighFreq::roll_var(matrix(taq$price), look_back=3, method="hampel")
> madv <- rutils::lagit(madv, lagg=-1, pad_zeros=FALSE)
> # Calculate Z-scores
> zscores <- ifelse(madv > 0, (taq$price - medianv)/madv, 0)
> range(zscores); mad(zscores)
> madv <- mad(zscores[abs(zscores)>0])
> hist(zscores, breaks=2000, xlim=c(-5*madv, 5*madv))
```



```
> # Define discrimination threshold value
> threshold <- 6*madv
> bad_ticks <- (abs(zscores) > threshold)
> good_ticks <- taq[!bad_ticks]
> # Calculate number of price jumps
> sum(bad_ticks)/NROW(zscores)
> # Coerce trade prices to xts
> xtsv <- xts::xts(good_ticks[, .(price, volume)], good_ticks$index)
> colnames(xtsv) <- c("XLK.Close", "XLK.Volume")
> # Plot dygraph of the clean lots
> dygraphs::dygraph(xtsv$XLK.Close,
+ main="XLK Trade Ticks for 2020-03-16 (Hampel filtered)")
> # Plot the large lots
> x11(width=6, height=5)
> quantmod::chart_Series(x=xtsv$XLK.Close,
+ name="XLK Trade Ticks for 2020-03-16 (Hampel filtered)")
```

Homework Assignment

Required

- Study all the lecture slides in *FRE6871_Lecture_5.pdf*, and run all the code in *FRE6871_Lecture_5.R*

Recommended

- Read about *PCA* in:
pca-handout.pdf
pcaTutorial.pdf
- Read about *optimization methods*:
Bolker Optimization Methods.pdf
Yollin Optimization.pdf
Boudt DEoptim Large Portfolio Optimization.pdf