Machine Learning

FRE6871 & FRE7241, Fall 2023

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January 27, 2024

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Vector and Matrix Calculus

Let $\mathbf{v}$ and $\mathbf{w}$ be vectors, with $\mathbf{v} = \{v_i\}_{i=1}^{i=n}$, and let $\mathbb{1}$ be the unit vector, with $\mathbb{1} = \{1\}_{i=1}^{i=n}$.

Then the inner product of $\mathbf{v}$ and $\mathbf{w}$ can be written as $\mathbf{v}^T\mathbf{w} = \mathbf{w}^T\mathbf{v} = \sum_{i=1}^{n} v_i w_i$.

We can then express the sum of the elements of $\mathbf{v}$ as the inner product: $\mathbf{v}^T\mathbb{1} = \mathbb{1}^T\mathbf{v} = \sum_{i=1}^{n} v_i$.

And the sum of squares of $\mathbf{v}$ as the inner product: $\mathbf{v}^T\mathbf{v} = \sum_{i=1}^{n} v_i^2$.

Let $\mathbb{A}$ be a matrix, with $\mathbb{A} = \{A_{ij}\}_{i,j=1}^{i,j=n}$.

Then the inner product of matrix $\mathbb{A}$ with vectors $\mathbf{v}$ and $\mathbf{w}$ can be written as:

$$\mathbf{v}^T\mathbb{A}\,\mathbf{w} = \mathbf{w}^T\mathbb{A}^T\mathbf{v} = \sum_{i,j=1}^{n} A_{ij} v_i w_j$$

The derivative of a scalar variable with respect to a vector variable is a vector, for example:

$$\frac{d(\mathbf{v}^T\mathbb{1})}{d\mathbf{v}} = d_v[\mathbf{v}^T\mathbb{1}] = d_v[\mathbb{1}^T\mathbf{v}] = \mathbb{1}^T$$

$$d_v[\mathbf{v}^T\mathbf{w}] = d_v[\mathbf{w}^T\mathbf{v}] = \mathbf{w}^T$$

$$d_v[\mathbf{v}^T\mathbb{A}\,\mathbf{w}] = \mathbf{w}^T\mathbb{A}^T$$

$$d_v[\mathbf{v}^T\mathbb{A}\,\mathbf{v}] = \mathbf{v}^T\mathbb{A} + \mathbf{v}^T\mathbb{A}^T$$

Eigenvectors and Eigenvalues of Matrices

The vector w is an *eigenvector* of the matrix $\mathbb{A}$, if it satisfies the *eigenvalue* equation:

$$\mathbb{A}\, w = \lambda\, w$$

Where λ is the *eigenvalue* corresponding to the *eigenvector* w.

The number of *eigenvalues* of a matrix is equal to its dimension.

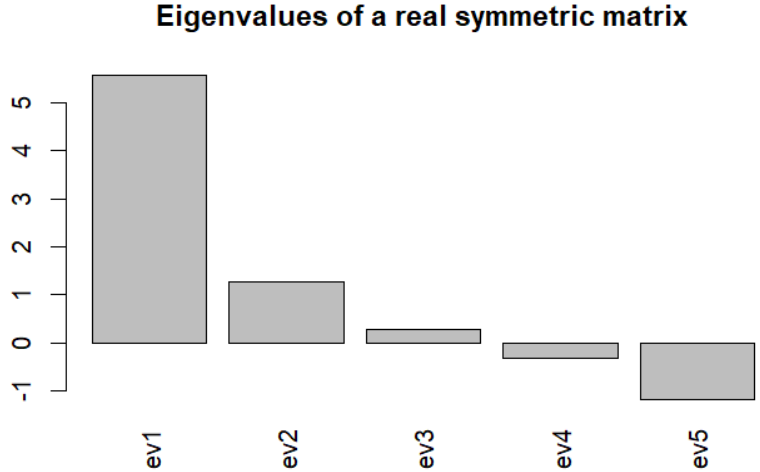
Real symmetric matrices have real *eigenvalues*, and their *eigenvectors* are orthogonal to each other.

The *eigenvectors* can be normalized to 1.

The *eigenvectors* form an *orthonormal basis* in which the matrix $\mathbb{A}$ is diagonal.

The function `eigen()` calculates the *eigenvectors* and *eigenvalues* of numeric matrices.

An excellent interactive visualization of *eigenvectors* and *eigenvalues* is available here:
http://setosa.io/ev/eigenvectors-and-eigenvalues/




```
> # Create a random real symmetric matrix
> matv <- matrix(runif(25), nc=5)
> matv <- matv + t(matv)
> # Calculate the eigenvalues and eigenvectors
> eigend <- eigen(matv)
> eigenvec <- eigend$vectors
> dim(eigenvec)
> # Plot eigenvalues
> barplot(eigend$values, xlab="", ylab="", las=3,
+   names.arg=paste0("ev", 1:NROW(eigend$values)),
+   main="Eigenvalues of a real symmetric matrix")
```

Eigen Decomposition of Matrices

Real symmetric matrices have real *eigenvalues*, and their *eigenvectors* are orthogonal to each other.

The *eigenvectors* form an *orthonormal basis* in which the matrix $\mathbb{A}$ is diagonal:

$$\Sigma = \mathbb{O}^T \mathbb{A} \mathbb{O}$$

Where Σ is a *diagonal* matrix containing the *eigenvalues* of matrix $\mathbb{A}$, and $\mathbb{O}$ is an *orthogonal* matrix of its *eigenvectors*, with $\mathbb{O}^T \mathbb{O} = \mathbb{1}$.

Any real symmetric matrix $\mathbb{A}$ can be decomposed into a product of its *eigenvalues* and its *eigenvectors* (the *eigen decomposition*):

$$\mathbb{A} = \mathbb{O} \Sigma \mathbb{O}^T$$

The *eigen decomposition* expresses a matrix as the product of a rotation, followed by a scaling, followed by the inverse rotation.

```
> # Eigenvectors form an orthonormal basis
> round(t(eigenvec) %*% eigenvec, digits=4)
> # Diagonalize matrix using eigenvector matrix
> round(t(eigenvec) %*% (matv %*% eigenvec), digits=4)
> eigend$values
> # Eigen decomposition of matrix by rotating the diagonal matrix
> matrixe <- eigenvec %*% (eigend$values * t(eigenvec))
> # Create diagonal matrix of eigenvalues
> # diagmat <- diag(eigend$values)
> # matrixe <- eigenvec %*% (diagmat %*% t(eigenvec))
> all.equal(matv, matrixe)
```

Orthogonal matrices represent rotations in *hyperspace*, and their inverse is equal to their transpose: $\mathbb{O}^{-1} = \mathbb{O}^T$.

The *diagonal* matrix Σ represents a scaling (stretching) transformation proportional to the *eigenvalues*.

The %*% operator performs *inner* (*scalar*) multiplication of vectors and matrices.

Inner multiplication multiplies the rows of one matrix with the columns of another matrix, so that each pair produces a single number.

Positive Definite Matrices

Matrices with positive *eigenvalues* are called *positive definite* matrices.

Matrices with non-negative *eigenvalues* are called *positive semi-definite* matrices (some of their *eigenvalues* may be zero).

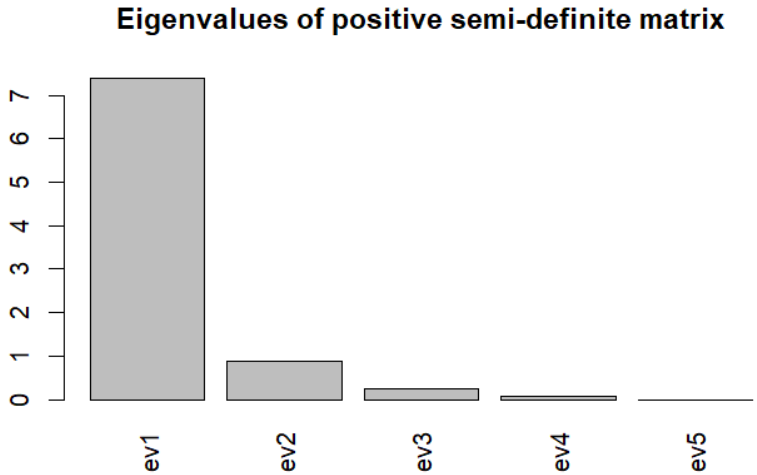
An example of *positive definite* matrices are the covariance matrices of linearly independent variables.

But the covariance matrices of linearly dependent variables have some *eigenvalues* equal to zero, in which case they are *singular*, and only *positive semi-definite*.

All covariance matrices are *positive semi-definite* and all *positive semi-definite* matrices are the covariance matrix of some multivariate distribution.

Matrices which have some *eigenvalues* equal to zero are called *singular* (degenerate) matrices.

For any real matrix $\mathbb{A}$, the matrix $\mathbb{A}^T\mathbb{A}$ is *positive semi-definite*.




```
> # Create a random positive semi-definite matrix
> matv <- matrix(runif(25), nc=5)
> matv <- t(matv) %*% matv
> # Calculate the eigenvalues and eigenvectors
> eigend <- eigen(matv)
> eigend$values
> # Plot eigenvalues
> barplot(eigend$values, las=3, xlab="", ylab="",
+   names.arg=paste0("ev", 1:NROW(eigend$values)),
+   main="Eigenvalues of positive semi-definite matrix")
```

Singular Value Decomposition (*SVD*) of Matrices

The *Singular Value Decomposition* (*SVD*) is a generalization of the *eigen decomposition* of square matrices.

The *SVD* of a rectangular matrix $\mathbb{A}$ is defined as the factorization:

$$\mathbb{A} = \mathbb{U}\,\mathbf{\Sigma}\,\mathbb{V}^T$$

Where $\mathbb{U}$ and $\mathbb{V}$ are the left and right *singular matrices*, and $\mathbf{\Sigma}$ is a diagonal matrix of *singular values*.

If $\mathbb{A}$ has `m` rows and `n` columns and if (`m > n`), then $\mathbb{U}$ is an (`m x n`) *rectangular* matrix, $\mathbf{\Sigma}$ is an (`n x n`) *diagonal* matrix, and $\mathbb{V}$ is an (`n x n`) *orthogonal* matrix, and if (`m < n`) then the dimensions are: (`m x m`), (`m x m`), and (`m x n`).

The left $\mathbb{U}$ and right $\mathbb{V}$ singular matrices consist of columns of *orthonormal* vectors, so that $\mathbb{U}^T\mathbb{U} = \mathbb{V}^T\mathbb{V} = \mathbb{1}$.

In the special case when $\mathbb{A}$ is a square matrix, then $\mathbb{U} = \mathbb{V}$, and the *SVD* reduces to the *eigen decomposition*.

The function `svd()` performs *Singular Value Decomposition* (*SVD*) of a rectangular matrix, and returns a list of three elements: the *singular values*, and the matrices of left-*singular* vectors and the right-*singular* vectors.

```
> # Perform singular value decomposition
> matv <- matrix(rnorm(50), nc=5)
> svdec <- svd(matv)
> # Recompose matv from SVD mat_rices
> all.equal(matv, svdec$u %*% (svdec$d*t(svdec$v)))
> # Columns of U and V are orthonormal
> round(t(svdec$u) %*% svdec$u, 4)
> round(t(svdec$v) %*% svdec$v, 4)
```

The Left and Right Singular Matrices

The left $\mathbb{U}$ and right $\mathbb{V}$ singular matrices define rotation transformations into a coordinate system where the matrix $\mathbb{A}$ becomes diagonal:

$$\mathbf{\Sigma} = \mathbb{U}^T \mathbb{A} \mathbb{V}$$

The columns of $\mathbb{U}$ and $\mathbb{V}$ are called the *singular* vectors, and they are only defined up to a reflection (change in sign), i.e. if vec is a singular vector, then so is -vec.

The left singular matrix $\mathbb{U}$ forms the *eigenvectors* of the matrix $\mathbb{A}\mathbb{A}^T$.

The right singular matrix $\mathbb{V}$ forms the *eigenvectors* of the matrix $\mathbb{A}^T\mathbb{A}$.

```
> # Dimensions of left and right matrices
> nrows <- 6 ; ncols <- 4
> # Calculate the left matrix
> leftmat <- matrix(runif(nrows^2), nc=nrows)
> eigend <- eigen(crossprod(leftmat))
> leftmat <- eigend$vectors[, 1:ncols]
> # Calculate the right matrix and singular values
> rightmat <- matrix(runif(ncols^2), nc=ncols)
> eigend <- eigen(crossprod(rightmat))
> rightmat <- eigend$vectors
> singval <- sort(runif(ncols, min=1, max=5), decreasing=TRUE)
> # Compose rectangular matrix
> matv <- leftmat %*% (singval * t(rightmat))
> # Perform singular value decomposition
> svdec <- svd(matv)
> # Recompose matv from SVD
> all.equal(matv, svdec$u %*% (svdec$d*t(svdec$v)))
> # Compare SVD with matv components
> all.equal(abs(svdec$u), abs(leftmat))
> all.equal(abs(svdec$v), abs(rightmat))
> all.equal(svdec$d, singval)
> # Eigen decomposition of matv squared
> retsq <- matv %*% t(matv)
> eigend <- eigen(retsq)
> all.equal(eigend$values[1:ncols], singval^2)
> all.equal(abs(eigend$vectors[, 1:ncols]), abs(leftmat))
> # Eigen decomposition of matv squared
> retsq <- t(matv) %*% matv
> eigend <- eigen(retsq)
> all.equal(eigend$values, singval^2)
> all.equal(abs(eigend$vectors), abs(rightmat))
```

Inverse of Symmetric Square Matrices

The inverse of a square matrix $\mathbb{A}$ is defined as a square matrix $\mathbb{A}^{-1}$ that satisfies the equation:

$$\mathbb{A}^{-1}\mathbb{A} = \mathbb{A}\mathbb{A}^{-1} = \mathbb{1}$$

Where $\mathbb{1}$ is the identity matrix.

The inverse $\mathbb{A}^{-1}$ of a *symmetric* square matrix $\mathbb{A}$ can also be expressed as the product of the inverse of its *eigenvalues* ($\mathbf{\Sigma}$) and its *eigenvectors* ($\mathbb{O}$):

$$\mathbb{A}^{-1} = \mathbb{O}\,\mathbf{\Sigma}^{-1}\,\mathbb{O}^{T}$$

But *singular* (degenerate) matrices (which have some *eigenvalues* equal to zero) don't have an inverse.

The inverse of *non-symmetric* matrices can be calculated using *Singular Value Decomposition* (*SVD*).

The function `solve()` solves systems of linear equations, and also inverts square matrices.

```
> # Create a random positive semi-definite matrix
> matv <- matrix(runif(25), nc=5)
> matv <- t(matv) %*% matv
> # Calculate the inverse of matv
> invmat <- solve(a=matv)
> # Multiply inverse with matrix
> round(invmat %*% matv, 4)
> round(matv %*% invmat, 4)
> # Calculate the eigenvalues and eigenvectors
> eigend <- eigen(matv)
> eigenvec <- eigend$vectors
> # Calculate the inverse from eigen decomposition
> inveigen <- eigenvec %*% (t(eigenvec) / eigend$values)
> all.equal(invmat, inveigen)
> # Decompose diagonal matrix with inverse of eigenvalues
> # diagmat <- diag(1/eigend$values)
> # inveigen <- eigenvec %*% (diagmat %*% t(eigenvec))
```

Generalized Inverse of Rectangular Matrices

The generalized inverse of an (`m x n`) rectangular matrix $\mathbb{A}$ is defined as an (`n x m`) matrix $\mathbb{A}^{-1}$ that satisfies the equation:

$$\mathbb{A}\mathbb{A}^{-1}\mathbb{A} = \mathbb{A}$$

The generalized inverse matrix $\mathbb{A}^{-1}$ can be expressed as a product of the inverse of its *singular values* ($\mathbf{\Sigma}$) and its left and right *singular* matrices ($\mathbb{U}$ and $\mathbb{V}$):

$$\mathbb{A}^{-1} = \mathbb{V}\mathbf{\Sigma}^{-1}\mathbb{U}^T$$

The generalized inverse $\mathbb{A}^{-1}$ can also be expressed as the *Moore-Penrose pseudo-inverse*:

$$\mathbb{A}^{-1} = (\mathbb{A}^T\mathbb{A})^{-1}\mathbb{A}^T$$

In the case when the inverse matrix $\mathbb{A}^{-1}$ exists, then the *pseudo-inverse* matrix simplifies to the inverse: $(\mathbb{A}^T\mathbb{A})^{-1}\mathbb{A}^T = \mathbb{A}^{-1}(\mathbb{A}^T)^{-1}\mathbb{A}^T = \mathbb{A}^{-1}$

The function `MASS::ginv()` calculates the generalized inverse of a matrix.

```
> # Random rectangular matrix: nrows > ncols
> nrows <- 6 ; ncols <- 4
> matv <- matrix(runif(nrows*ncols), nc=ncols)
> # Calculate the generalized inverse of matv
> invmat <- MASS::ginv(matv)
> round(invmat %*% matv, 4)
> all.equal(matv, matv %*% invmat %*% matv)
> # Random rectangular matrix: nrows < ncols
> nrows <- 4 ; ncols <- 6
> matv <- matrix(runif(nrows*ncols), nc=ncols)
> # Calculate the generalized inverse of matv
> invmat <- MASS::ginv(matv)
> all.equal(matv, matv %*% invmat %*% matv)
> round(matv %*% invmat, 4)
> round(invmat %*% matv, 4)
> # Perform singular value decomposition
> svdec <- svd(matv)
> # Calculate the generalized inverse from SVD
> invsvd <- svdec$v %*% (t(svdec$u) / svdec$d)
> all.equal(invsvd, invmat)
> # Calculate the Moore-Penrose pseudo-inverse
> invmp <- MASS::ginv(t(matv) %*% matv) %*% t(matv)
> all.equal(invmp, invmat)
```

Regularized Inverse of Singular Matrices

Singular matrices have some *singular values* equal to zero, so they don't have an inverse matrix which satisfies the equation: $\mathbb{A}\mathbb{A}^{-1}\mathbb{A} = \mathbb{A}$

But if the *singular values* that are equal to zero are removed, then a *regularized inverse* for *singular* matrices can be specified by:

$$\mathbb{A}^{-1} = \mathbb{V}_n \, \mathbf{\Sigma}_n^{-1} \, \mathbb{U}_n^T$$

Where $\mathbb{U}_n$, $\mathbb{V}_n$ and $\mathbf{\Sigma}_n$ are the *SVD* matrices with the rows and columns corresponding to zero *singular values* removed.

```
> # Create a random singular matrix
> # More columns than rows: ncols > nrows
> nrows <- 4 ; ncols <- 6
> matv <- matrix(runif(nrows*ncols), nc=ncols)
> matv <- t(matv) %*% matv
> # Perform singular value decomposition
> svdec <- svd(matv)
> # Incorrect inverse from SVD because of zero singular values
> invsvd <- svdec$v %*% (t(svdec$u) / svdec$d)
> # Inverse property doesn't hold
> all.equal(matv, matv %*% invsvd %*% matv)
```

```
> # Set tolerance for determining zero singular values
> precv <- sqrt(.Machine$double.eps)
> # Check for zero singular values
> round(svdec$d, 12)
> notzero <- (svdec$d > (precv*svdec$d[1]))
> # Calculate the regularized inverse from SVD
> invsvd <- svdec$v[, notzero] %*%
+   (t(svdec$u[, notzero]) / svdec$d[notzero])
> # Verify inverse property of matv
> all.equal(matv, matv %*% invsvd %*% matv)
> # Calculate the regularized inverse using MASS::ginv()
> invmat <- MASS::ginv(matv)
> all.equal(invsvd, invmat)
> # Calculate the Moore-Penrose pseudo-inverse
> invmp <- MASS::ginv(t(matv) %*% matv) %*% t(matv)
> all.equal(invmp, invmat)
```

Diagonalizing the Inverse of Singular Matrices

The left-*singular* matrix $\mathbb{U}$ combined with the right-*singular* matrix $\mathbb{V}$ define a rotation transformation into a coordinate system where the matrix $\mathbb{A}$ becomes diagonal:

$$\mathbf{\Sigma} = \mathbb{U}^T \mathbb{A} \mathbb{V}$$

The generalized inverse of *singular* matrices doesn't satisfy the equation: $\mathbb{A}^{-1}\mathbb{A} = \mathbb{A}\mathbb{A}^{-1} = \mathbb{1}$, but if it's rotated into the same coordinate system where $\mathbb{A}$ is diagonal, then we have:

$$\mathbb{U}^T (\mathbb{A}^{-1}\mathbb{A}) \mathbb{V} = \mathbb{1}_n$$

So that $\mathbb{A}^{-1}\mathbb{A}$ is diagonal in the same coordinate system where $\mathbb{A}$ is diagonal.

```
> # Diagonalize the unit matrix
> unitmat <- matv %*% invmat
> round(unitmat, 4)
> round(matv %*% invmat, 4)
> round(t(svdec$u) %*% unitmat %*% svdec$v, 4)
```

Solving Linear Equations Using solve()

A system of linear equations can be defined as:

$$\mathbb{A}\,x = b$$

Where $\mathbb{A}$ is a matrix, b is a vector, and x is the unknown vector.

The solution of the system of linear equations is equal to:

$$x = \mathbb{A}^{-1} b$$

Where $\mathbb{A}^{-1}$ is the *inverse* of the matrix $\mathbb{A}$.

The function `solve()` solves systems of linear equations, and also inverts square matrices.

The %*% operator performs *inner* (*scalar*) multiplication of vectors and matrices.

Inner multiplication multiplies the rows of one matrix with the columns of another matrix, so that each pair produces a single number:

```
> # Define a square matrix
> matv <- matrix(c(1, 2, -1, 2), nc=2)
> vecv <- c(2, 1)
> # Calculate the inverse of matv
> invmat <- solve(a=matv)
> invmat %*% matv
> # Calculate the solution using inverse of matv
> solutionv <- invmat %*% vecv
> matv %*% solutionv
> # Calculate the solution of linear system
> solutionv <- solve(a=matv, b=vecv)
> matv %*% solutionv
```

Fast Matrix Inverse Using C++

The *Armadillo* C++ functions can be several times faster than R functions - even those that are compiled from C++ code.

That's because the *Armadillo* C++ library calls routines optimized for fast numerical calculations.

The package *RcppArmadillo* allows calling from R the high-level *Armadillo* C++ linear algebra library.

The C++ *Armadillo* function `arma::inv()` calculates the matrix inverse several times faster than the function `solve()`.

The function `solve()` calculates the matrix inverse several times faster than the function `MASS::ginv()`.

```
> # Create a random matrix
> matv <- matrix(rnorm(100), nc=10)
> # Calculate the matrix inverse using solve()
> invmatr <- solve(a=matv)
> round(invmatr %*% matv, 4)
> # Compile the C++ file using Rcpp
> Rcpp::sourceCpp(file="/Users/jerzy/Develop/Rcpp/test_fun.cpp")
> # Calculate the matrix inverse using C++
> invmat <- calc_invmat(matv)
> all.equal(invmat, invmatr)
> # Compare the speed of RcppArmadillo with R code
> library(microbenchmark)
> summary(microbenchmark(
+   ginv=MASS::ginv(matv),
+   solve=solve(matv),
+   cpp=calc_invmat(matv),
+   times=10))[, c(1, 4, 5)]
```

```
// Rcpp header with information for C++ compiler
// [[Rcpp::depends(RcppArmadillo)]]
#include <RcppArmadillo.h> // include RcppArmadillo header file
using namespace arma; // use Armadillo C++ namespace

// [[Rcpp::export]]
arma::mat calc_invmat(arma::mat& matv) {

  return arma::inv(matv);

}  // end calc_invmat
```

Cholesky Decomposition

The *Cholesky* decomposition of a *positive definite* matrix $\mathbb{A}$ is defined as:

$$\mathbb{A} = \mathbb{L}^T \mathbb{L}$$

Where $\mathbb{L}$ is an upper triangular matrix with positive diagonal elements.

The matrix $\mathbb{L}$ can be considered the square root of $\mathbb{A}$.

The vast majority of random *positive semi-definite* matrices are also *positive definite*.

The function `chol()` calculates the *Cholesky* decomposition of a *positive definite* matrix.

The functions `chol2inv()` and `chol()` calculate the inverse of a *positive definite* matrix two times faster than `solve()`.

```
> # Create large random positive semi-definite matrix
> matv <- matrix(runif(1e4), nc=100)
> matv <- t(matv) %*% matv
> # Calculate the eigen decomposition
> eigend <- eigen(matv)
> eigenval <- eigend$values
> eigenvec <- eigend$vectors
> # Set tolerance for determining zero singular values
> precv <- sqrt(.Machine$double.eps)
> # If needed convert to positive definite matrix
> notzero <- (eigenval > (precv*eigenval[1]))
> if (sum(!notzero) > 0) {
+   eigenval[!notzero] <- 2*precv
+   matv <- eigenvec %*% (eigenval * t(eigenvec))
+ }  # end if
> # Calculate the Cholesky matv
> cholmat <- chol(matv)
> cholmat[1:5, 1:5]
> all.equal(matv, t(cholmat) %*% cholmat)
> # Calculate the inverse from Cholesky
> invchol <- chol2inv(cholmat)
> all.equal(solve(matv), invchol)
> # Compare speed of Cholesky inversion
> library(microbenchmark)
> summary(microbenchmark(
+   solve=solve(matv),
+   cholmat=chol2inv(chol(matv)),
+   times=10))[, c(1, 4, 5)]  # end microbenchmark summary
```

Simulating Correlated Returns Using Cholesky Matrix

The *Cholesky* decomposition of a covariance matrix can be used to simulate correlated *Normal* returns following the given covariance matrix: $\mathbb{C} = \mathbb{L}^T\mathbb{L}$

Let $\mathbb{R}$ be a matrix with columns of *uncorrelated* returns following the *Standard Normal* distribution.

The *correlated* returns $\mathbb{R}_c$ can be calculated from the *uncorrelated* returns $\mathbb{R}$ by multiplying them by the *Cholesky* matrix $\mathbb{L}$:

$$\mathbb{R}_c = \mathbb{L}^T\mathbb{R}$$

```
> # Calculate the random covariance matrix
> covmat <- matrix(runif(25), nc=5)
> covmat <- t(covmat) %*% covmat
> # Calculate the Cholesky matrix
> cholmat <- chol(covmat)
> cholmat
> # Simulate random uncorrelated returns
> nassets <- 5
> nrows <- 10000
> retp <- matrix(rnorm(nassets*nrows), nc=nassets)
> # Calculate the correlated returns by applying Cholesky
> retscorr <- retp %*% cholmat
> # Calculate the covariance matrix
> covmat2 <- crossprod(retscorr) /(nrows-1)
> all.equal(covmat, covmat2)
```

Eigenvalues of Singular Covariance Matrices

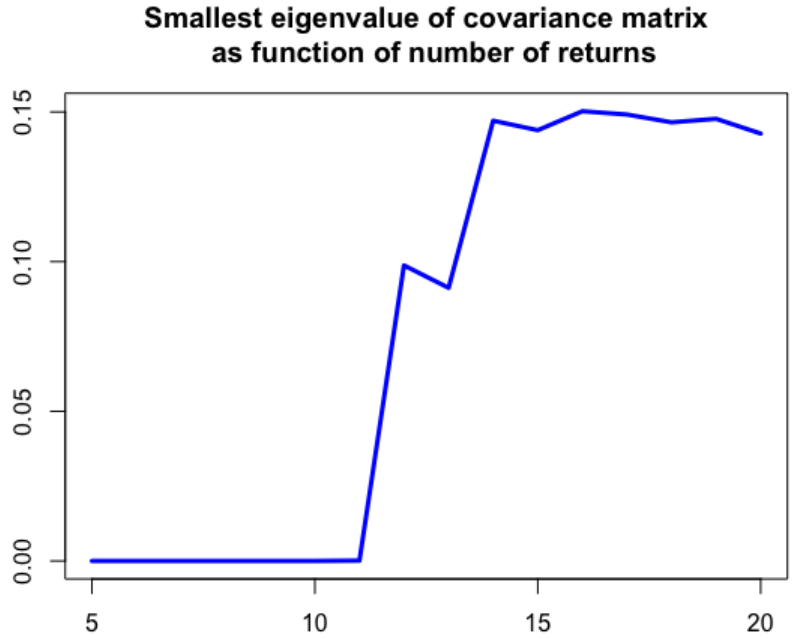
If $\mathbb{R}$ is a matrix of returns (with zero mean) for a portfolio of `k` stocks (columns), over `n` time periods (rows), then the sample covariance matrix is equal to:

$$\mathbb{C} = \mathbb{R}^T \mathbb{R}/(n-1)$$

If the number of rows is less than the number of stocks, then the returns are *collinear*, and the sample covariance matrix is *singular*, with some *eigenvalues* equal to zero.

The function `crossprod()` performs *inner* (*scalar*) multiplication, exactly the same as the %*% operator, but it is slightly faster.

```
> # Simulate random stock returns
> nassets <- 10
> nrows <- 100
> # Initialize the random number generator
> set.seed(1121, "Mersenne-Twister", sample.kind="Rejection")
> retp <- matrix(rnorm(nassets*nrows), nc=nassets)
> # Calculate the centered (de-meaned) returns matrix
> retp <- t(t(retp) - colMeans(retp))
> # Or
> retp <- apply(retp, MARGIN=2, function(x) (x-mean(x)))
> # Calculate the covariance matrix
> covmat <- crossprod(retp) /(nrows-1)
> # Calculate the eigenvalues and eigenvectors
> eigend <- eigen(covmat)
> eigend$values
> barplot(eigend$values, # Plot eigenvalues
+   xlab="", ylab="", las=3,
+   names.arg=paste0("ev", 1:NROW(eigend$values)),
+   main="Eigenvalues of Covariance Matrix")
```




```
> # Calculate the eigenvalues and eigenvectors
> # as function of number of returns
> ndata <- ((nassets/2):(2*nassets))
> eigenval <- sapply(ndata, function(x) {
+   retp <- retp[1:x, ]
+   retp <- apply(retp, MARGIN=2, function(y) (y - mean(y)))
+   covmat <- crossprod(retp) / (x-1)
+   min(eigen(covmat)$values)
+ })  # end sapply
> plot(y=eigenval, x=ndata, t="l", xlab="", ylab="", lwd=3, col="blu
+   main="Smallest eigenvalue of covariance matrix
+   as function of number of returns")
```

Regularized Inverse of Singular Covariance Matrices

The *regularization* technique allows calculating the inverse of *singular* covariance matrices while reducing the effects of statistical noise.

If the number of time periods of returns is less than the number of assets (columns), then the covariance matrix of returns is *singular*, and some of its *eigenvalues* are zero, so it doesn't have an inverse.

The *regularized* inverse $\mathbb{C}_n^{-1}$ is calculated by removing the higher order eigenvalues that are almost zero, and keeping only the first *n eigenvalues*:

$$\mathbb{C}_n^{-1} = \mathbb{O}_n \, \mathbf{\Sigma}_n^{-1} \, \mathbb{O}_n^T$$

Where $\mathbf{\Sigma}_n$ and $\mathbb{O}_n$ are matrices with the higher order eigenvalues and eigenvectors removed.

The function `MASS::ginv()` calculates the *regularized* inverse of a matrix.

```
> # Create rectangular matrix with collinear columns
> matv <- matrix(rnorm(10*8), nc=10)
> # Calculate the covariance matrix
> covmat <- cov(matv)
> # Calculate the inverse of covmat - error
> invmat <- solve(covmat)
> # Calculate the regularized inverse of covmat
> invmat <- MASS::ginv(covmat)
> # Verify inverse property of matv
> all.equal(covmat, covmat %*% invmat %*% covmat)
> # Perform eigen decomposition
> eigend <- eigen(covmat)
> eigenvec <- eigend$vectors
> eigenval <- eigend$values
> # Set tolerance for determining zero singular values
> precv <- sqrt(.Machine$double.eps)
> # Calculate the regularized inverse matrix
> notzero <- (eigenval > (precv * eigenval[1]))
> invreg <- eigenvec[, notzero] %*%
+   (t(eigenvec[, notzero]) / eigenval[notzero])
> # Verify that invmat is same as invreg
> all.equal(invmat, invreg)
```

The Bias-Variance Tradeoff of the Regularized Inverse

Removing the very small higher order eigenvalues can also be used to reduce the propagation of statistical noise and improve the signal-to-noise ratio.

Removing a larger number of eigenvalues further reduces the noise, but it increases the bias of the covariance matrix.

This is an example of the *bias-variance tradeoff*.

Even though the *regularized* inverse $\mathbb{C}_n^{-1}$ does not satisfy the matrix inverse property, its out-of-sample forecasts may be more accurate than those using the actual inverse matrix.

The parameter `dimax` specifies the number of eigenvalues used for calculating the *regularized* inverse of the covariance matrix of returns.

The optimal value of the parameter `dimax` can be determined using *backtesting* (*cross-validation*).

```
> # Calculate the regularized inverse matrix using cutoff
> dimax <- 3
> invmat <- eigenvec[, 1:dimax] %*%
+   (t(eigenvec[, 1:dimax]) / eigend$values[1:dimax])
> # Verify that invmat is same as invreg
> all.equal(invmat, invreg)
```

Shrinkage Estimator of Covariance Matrices

The estimates of the covariance matrix suffer from statistical noise, and those noise are magnified when the covariance matrix is inverted.

In the *shrinkage* technique the covariance matrix $\mathbb{C}_s$ is estimated as a weighted sum of the sample covariance estimator $\mathbb{C}$ plus a target matrix $\mathbb{T}$:

$$\mathbb{C}_s = (1 - \alpha)\,\mathbb{C} + \alpha\,\mathbb{T}$$

The target matrix $\mathbb{T}$ represents an estimate of the covariance matrix subject to some constraint, such as that all the correlations are equal to each other.

The shrinkage intensity α determines the amount of shrinkage that is applied, with $\alpha = 1$ representing a complete shrinkage towards the target matrix.

The *shrinkage* estimator reduces the estimate variance at the expense of increasing its bias (known as the *bias-variance tradeoff*).

```
> # Create a random covariance matrix
> set.seed(1121, "Mersenne-Twister", sample.kind="Rejection")
> matv <- matrix(rnorm(5e2), nc=5)
> covmat <- cov(matv)
> cormat <- cor(matv)
> stdev <- sqrt(diag(covmat))
> # Calculate the target matrix
> cormean <- mean(cormat[upper.tri(cormat)])
> targetmat <- matrix(cormean, nr=NROW(covmat), nc=NCOL(covmat))
> diag(targetmat) <- 1
> targetmat <- t(t(targetmat * stdev) * stdev)
> # Calculate the shrinkage covariance matrix
> alphac <- 0.5
> covshrink <- (1-alphac)*covmat + alphac*targetmat
> # Calculate the inverse matrix
> invmat <- solve(covshrink)
```

Recursive Matrix Inverse

The inverse of a square matrix $\mathbb{A}$ can be calculated approximately using the recursive *Schulz formula*:

$$\mathbb{A}_{i+1}^{-1} \leftarrow 2\mathbb{A}_i^{-1} - \mathbb{A}_i^{-1}\mathbb{A}\mathbb{A}_i^{-1}$$

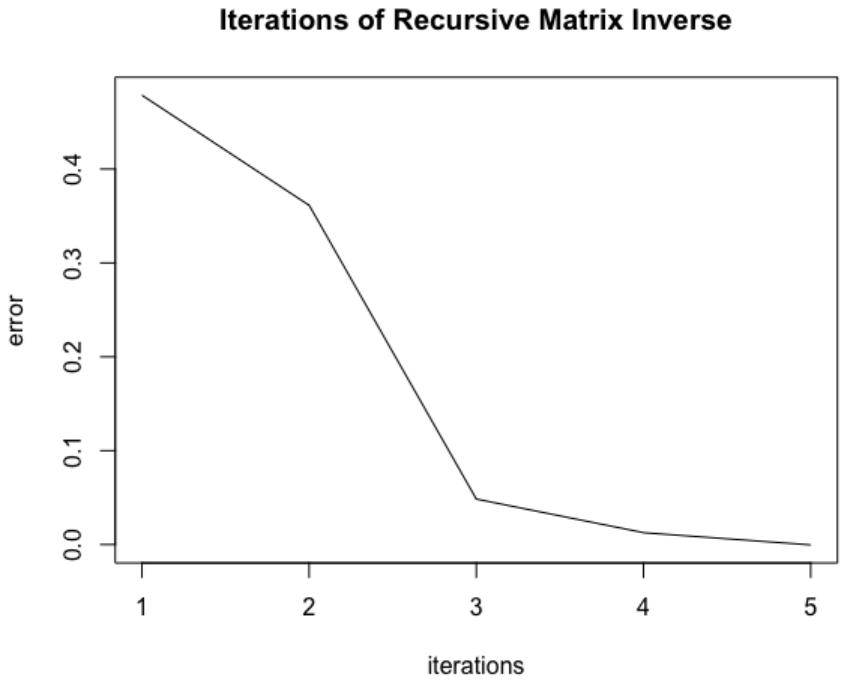
The *Schulz formula* requires a good initial value for the inverse matrix $\mathbb{A}_1^{-1}$ or else the recursion diverges.

If the initial inverse matrix $\mathbb{A}_1^{-1}$ is very close to the actual inverse $\mathbb{A}^{-1}$, then the *Schulz formula* produces a very good approximation with just a few iterations.

The *Schulz formula* is useful for updating the inverse when the matrix $\mathbb{A}$ changes only slightly. For example, for updating the inverse of the covariance matrix as it changes slowly over time.

The super-assignment operator "<<-" modifies variables in the *enclosing* environment in which the function was *defined* (*lexical* scoping).

```
> # Create a random matrix
> matv <- matrix(rnorm(100), nc=10)
> # Calculate the inverse of matv
> invmat <- solve(a=matv)
> # Multiply inverse with matrix
> round(invmat %*% matv, 4)
> # Calculate the initial inverse
> invmatr <- invmat + matrix(rnorm(100, sd=0.1), nc=10)
> # Calculate the approximate recursive inverse of matv
> invmatr <- (2*invmatr - invmatr %*% matv %*% invmatr)
> # Calculate the sum of the off-diagonal elements
> sum((invmatr %*% matv)[upper.tri(matv)])
```




```
> # Calculate the recursive inverse of matv in a loop
> invmatr <- invmat + matrix(rnorm(100, sd=0.1), nc=10)
> iterv <- sapply(1:5, function(x) {
+ # Calculate the recursive inverse of matv
+   invmatr <<- (2*invmatr - invmatr %*% matv %*% invmatr)
+ # Calculate the sum of the off-diagonal elements
+   sum((invmatr %*% matv)[upper.tri(matv)])
+ })  # end sapply
> # Plot the iterations
> plot(x=1:5, y=iterv, t="l", xlab="iterations", ylab="error",
+      main="Iterations of Recursive Matrix Inverse")
```

draft: Principal Components of Two Stocks

The scaled returns of *XLP* and *VTI* can be expressed as linear combinations of two orthogonal principal components:
The first principal component can be returns of *XLP* and *VTI* are highly correlated because they both share a common factor of market returns.

```
> # Perform PCA for two stocks
> retp <- scale(na.omit(rutils::etfenv$returns
+           [, as.character(formulav)[-1]]))
> crossprod(retp) / NROW(retp)
> w1 <- sqrt(0.5); w2 <- w1
> foo <- matrix(c(w1, w2, -w2, w1), nc=2)
> t(foo) %*% foo
> # bar <- retp %*% t(solve(foo))
> (t(bar) %*% bar) / NROW(bar)
>
> covmat <- function(retp, anglev=0) {
+   w1 <- cos(anglev)
+   w2 <- sin(anglev)
+   matv <- matrix(c(w1, -w2, w2, w1), nc=2)
+   pcav <- retp %*% t(matv)
+   (t(pcav) %*% pcav) / NROW(pcav)
+ }  # end covmat
>
> bar <- covmat(retp, anglev=pi/4)
> crossprod(retp) / NROW(retp)
> (t(bar) %*% bar) / NROW(bar)
>
> angles <- seq(0, pi/2, by=pi/24)
> covmat <- sapply(angles, function(anglev)
+   covmat(retp, anglev=anglev)[1, 1])
> plot(x=angles, y=covmat, t="l")
>
> optiml <- optimize(
+   f=function(anglev)
```

```
> # Plot scatterplot of returns
> plot(formulav, data=rutils::etfenv$returns,
+      main="Regression XLP ~ VTI")
> # Add regression line
> abline(regmod, lwd=2, col="red")
```

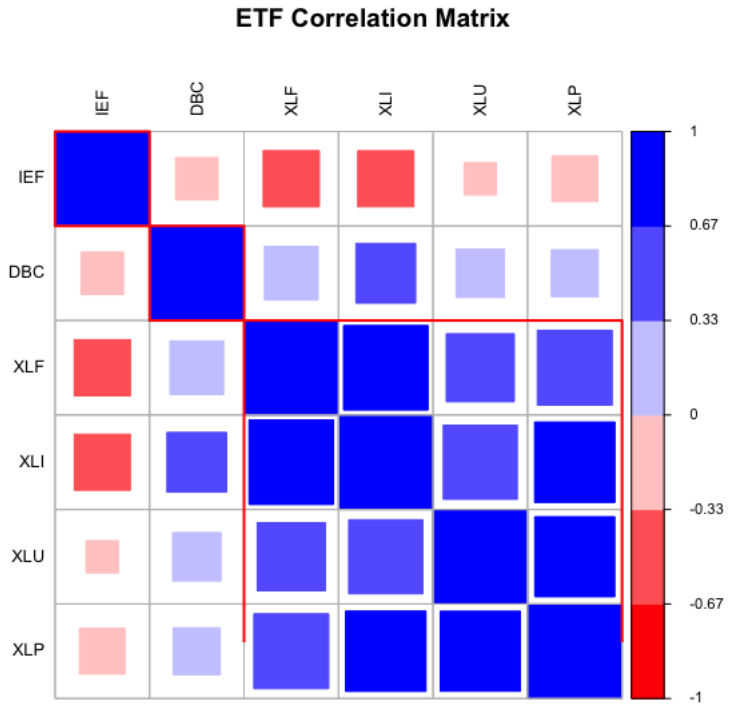
Covariance Matrix of ETF Returns

The covariance matrix $\mathbb{C}$, of the return matrix $\mathbf{r}$ is given by:

$$\mathbb{C} = \frac{(\mathbf{r} - \bar{\mathbf{r}})^T (\mathbf{r} - \bar{\mathbf{r}})}{n - 1}$$

If the returns are *standardized* (centered and scaled) then the covariance matrix is equal to the correlation matrix.

```
> # Select ETF symbols
> symbolv <- c("IEF", "DBC", "XLU", "XLF", "XLP", "XLI")
> # Calculate the ETF prices and log returns
> pricev <- rutils::etfenv$prices[, symbolv]
> # Applying zoo::na.locf() can produce bias of the correlations
> # pricev <- zoo::na.locf(pricev, na.rm=FALSE)
> # pricev <- zoo::na.locf(pricev, fromLast=TRUE)
> pricev <- na.omit(pricev)
> retp <- rutils::diffit(log(pricev))
> # Calculate the covariance matrix
> covmat <- cov(retp)
> # Standardize (de-mean and scale) the returns
> retp <- lapply(retp, function(x) {(x - mean(x))/sd(x)})
> retp <- rutils::do_call(cbind, retp)
> round(sapply(retp, mean), 6)
> sapply(retp, sd)
> # Alternative (much slower) center (de-mean) and scale the retur
> # retp <- apply(retp, 2, scale)
> # retp <- xts::xts(retp, zoo::index(pricev))
> # Alternative (much slower) center (de-mean) and scale the retur
> # retp <- scale(retp, center=TRUE, scale=TRUE)
> # retp <- xts::xts(retp, zoo::index(pricev))
> # Alternative (much slower) center (de-mean) and scale the retur
> # retp <- t(retp) - colMeans(retp)
> # retp <- retp/sqrt(rowSums(retp^2)/(NCOL(retp)-1))
> # retp <- t(retp)
```




```
> # Calculate the correlation matrix
> cormat <- cor(retp)
> # Reorder correlation matrix based on clusters
> library(corrplot)
> ordern <- corrMatOrder(cormat, order="hclust",
+   hclust.method="complete")
> cormat <- cormat[ordern, ordern]
> # Plot the correlation matrix
> colorv <- colorRampPalette(c("red", "white", "blue"))
> # x11(width=6, height=6)
> corrplot(cormat, title=NA, tl.col="black", mar=c(0,0,0,0),
+     method="square", col=colorv(NCOL(cormat)), tl.cex=0.8,
+     cl.offset=0.75, cl.cex=0.7, cl.align.text="l", cl.ratio=0.25)
```

Principal Component Vectors

Principal components are linear combinations of the k return vectors $\mathbf{r}_i$:

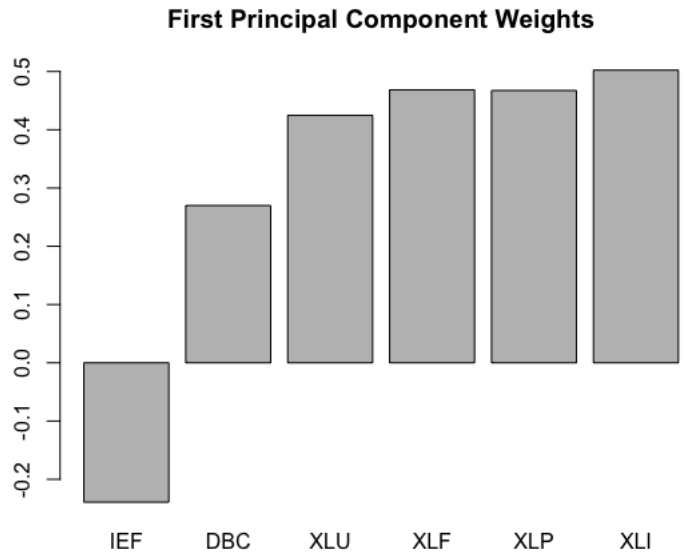
$$\mathbf{pc}_j = \sum_{i=1}^{k} w_{ij}\, \mathbf{r}_i$$

Where $\mathbf{w}_j$ is a vector of weights (loadings) of the *principal component* j, with $\mathbf{w}_j^T \mathbf{w}_j = 1$.

The weights $\mathbf{w}_j$ are chosen to maximize the variance of the *principal components*, under the condition that they are orthogonal:

$$\mathbf{w}_j = \arg\max \left\{ \mathbf{pc}_j^T\, \mathbf{pc}_j \right\}$$

$$\mathbf{pc}_i^T\, \mathbf{pc}_j = 0 \; (i \neq j)$$




```
> # Create initial vector of portfolio weights
> nweights <- NROW(symbolv)
> weightv <- rep(1/sqrt(nweights), nweights)
> names(weightv) <- symbolv
> # Objective function equal to minus portfolio variance
> objfun <- function(weightv, retp) {
+   retp <- retp %*% weightv
+   -sum(retp^2) + 1e4*(1 - sum(weightv^2))^2
+ }  # end objfun
> # Objective for equal weight portfolio
> objfun(weightv, retp)
> # Compare speed of vector multiplication methods
> summary(microbenchmark(
+   transp=(t(retp[, 1]) %*% retp[, 1]),
+   sumv=sum(retp[, 1]^2),
+   times=10))[, c(1, 4, 5)]
```

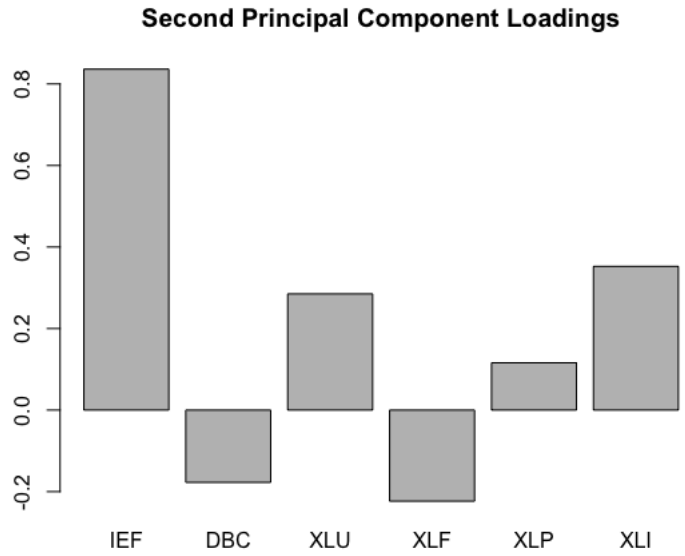
```
> # Find weights with maximum variance
> optim1 <- optim(par=weightv,
+   fn=objfun,
+   retp=retp,
+   method="L-BFGS-B",
+   upper=rep(10.0, nweights),
+   lower=rep(-10.0, nweights))
> # Optimal weights and maximum variance
> weights1 <- optim1$par
> -objfun(weights1, retp)
> # Plot first principal component weights
> barplot(weights1, names.arg=names(weights1), xlab="", ylab="",
+   main="First Principal Component Weights")
```

Higher Order Principal Components

The second *principal component* can be calculated by maximizing its variance, under the constraint that it must be orthogonal to the first *principal component*.

Similarly, higher order *principal components* can be calculated by maximizing their variances, under the constraint that they must be orthogonal to all the previous *principal components*.

```
> # PC1 returns
> pc1 <- drop(retp %*% weights1)
> # Redefine objective function
> objfun <- function(weightv, retp) {
+   retp <- retp %*% weightv
+   -sum(retp^2) + 1e4*(1 - sum(weightv^2))^2 +
+     1e4*(sum(weights1*weightv))^2
+ }  # end objfun
> # Find second PC weights using parallel DEoptim
> optim1 <- DEoptim::DEoptim(fn=objfun,
+   upper=rep(10, NCOL(retp)),
+   lower=rep(-10, NCOL(retp)),
+   retp=retp, control=list(parVar="weights1",
+     trace=FALSE, itermax=1000, parallelType=1))
```




```
> # PC2 weights
> weights2 <- optim1$optim$bestmem
> names(weights2) <- colnames(retp)
> sum(weights2^2)
> sum(weights1*weights2)
> # PC2 returns
> pc2 <- drop(retp %*% weights2)
> # Plot second principal component loadings
> barplot(weights2, names.arg=names(weights2), xlab="", ylab="",
+   main="Second Principal Component Loadings")
```

Eigenvalues of the Correlation Matrix

The portfolio variance: $\mathbf{w}^T \mathbb{C} \mathbf{w}$ can be maximized under the *quadratic* weights constraint $\mathbf{w}^T \mathbf{w} = 1$, by maximizing the *Lagrangian* $\mathcal{L}$:

$$\mathcal{L} = \mathbf{w}^T \mathbb{C} \mathbf{w} - \lambda (\mathbf{w}^T \mathbf{w} - 1)$$

Where λ is a *Lagrange multiplier*.

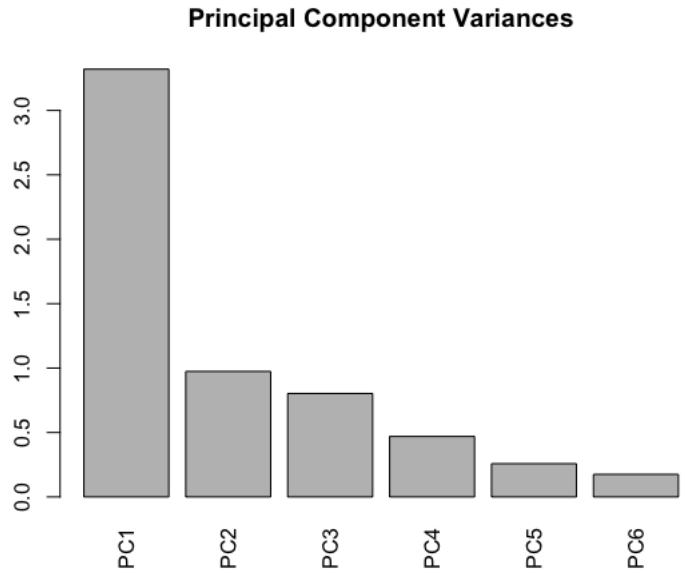
The maximum variance portfolio weights can be found by differentiating $\mathcal{L}$ with respect to $\mathbf{w}$ and setting it to zero:

$$\mathbb{C} \mathbf{w} = \lambda \mathbf{w}$$

This is the *eigenvalue* equation of the covariance matrix $\mathbb{C}$, with the optimal weights $\mathbf{w}$ forming an *eigenvector*, and λ is the *eigenvalue* corresponding to the *eigenvector* $\mathbf{w}$.

The *eigenvalues* are the variances of the *eigenvectors*, and their sum is equal to the sum of the return variances:

$$\sum_{i=1}^{k} \lambda_i = \frac{1}{1-k} \sum_{i=1}^{k} \mathbf{r}_i^T \mathbf{r}_i$$




```
> # Calculate the eigenvalues and eigenvectors
> eigend <- eigen(cormat)
> eigend$vectors
> # Compare with optimization
> all.equal(sum(diag(cormat)), sum(eigend$values))
> all.equal(abs(eigend$vectors[, 1]), abs(weights1), check.attribute
> all.equal(abs(eigend$vectors[, 2]), abs(weights2), check.attribute
> all.equal(eigend$values[1], var(pc1), check.attributes=FALSE)
> all.equal(eigend$values[2], var(pc2), check.attributes=FALSE)
> # Eigenvalue equations
> (cormat %*% weights1) / weights1 / var(pc1)
> (cormat %*% weights2) / weights2 / var(pc2)
> # Plot eigenvalues
> barplot(eigend$values, names.arg=paste0("PC", 1:nweights),
+   las=3, xlab="", ylab="", main="Principal Component Variances")
```

Principal Component Analysis Versus *Eigen Decomposition*

Principal Component Analysis (*PCA*) is equivalent to the *eigen decomposition* of either the correlation or the covariance matrix.

If the input time series *are* scaled, then *PCA* is equivalent to the eigen decomposition of the *correlation matrix*.

If the input time series *are not* scaled, then *PCA* is equivalent to the eigen decomposition of the *covariance matrix*.

Scaling the input time series improves the accuracy of the *PCA dimension reduction*, allowing a smaller number of *principal components* to more accurately capture the data contained in the input time series.

The number of *eigenvalues* is equal to the dimension of the covariance matrix.

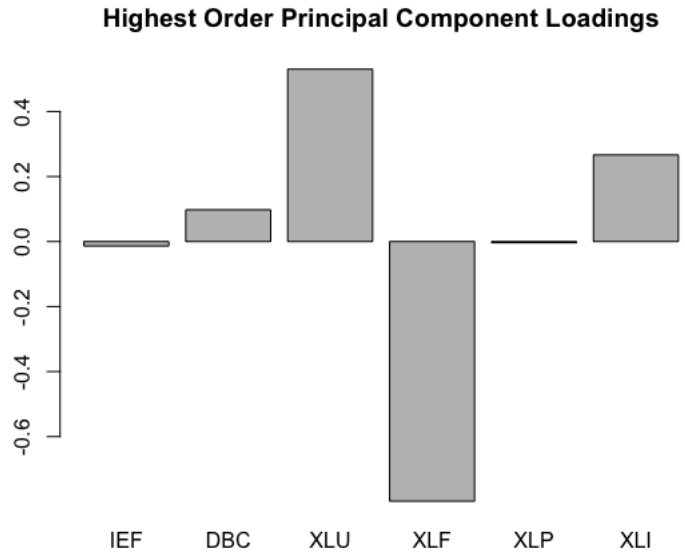
```
> # Calculate the eigen decomposition of the correlation matrix
> eigend <- eigen(cormat)
> # Perform PCA with scaling
> pcad <- prcomp(retp, scale=TRUE)
> # Compare outputs
> all.equal(eigend$values, pcad$sdev^2)
> all.equal(abs(eigend$vectors), abs(pcad$rotation),
+     check.attributes=FALSE)
> # Eigen decomposition of covariance matrix
> eigend <- eigen(covmat)
> # Perform PCA without scaling
> pcad <- prcomp(retp, scale=FALSE)
> # Compare outputs
> all.equal(eigend$values, pcad$sdev^2)
> all.equal(abs(eigend$vectors), abs(pcad$rotation),
+     check.attributes=FALSE)
```

Minimum Variance Portfolio

The highest order *principal component*, with the smallest eigenvalue, has the lowest possible variance, under the *quadratic* weights constraint: $\mathbf{w}^T\mathbf{w} = 1$.

So the highest order *principal component* is equal to the *Minimum Variance Portfolio*.

```
> # Redefine objective function to minimize variance
> objfun <- function(weightv, retp) {
+   retp <- retp %*% weightv
+   sum(retp^2) + 1e4*(1 - sum(weightv^2))^2
+ }  # end objfun
> # Find highest order PC weights using parallel DEoptim
> optiml <- DEoptim::DEoptim(fn=objfun,
+   upper=rep(10, NCOL(retp)),
+   lower=rep(-10, NCOL(retp)),
+   retp=retp, control=list(trace=FALSE,
+     itermax=1000, parallelType=1))
> # PC6 weights and returns
> weights6 <- optiml$optim$bestmem
> names(weights6) <- colnames(retp)
> sum(weights6^2)
> sum(weights1*weights6)
> # Compare with eigend vector
> weights6
> eigend$vectors[, 6]
> # Calculate the objective function
> objfun(weights6, retp)
> objfun(eigend$vectors[, 6], retp)
```




```
> # Plot highest order principal component loadings
> weights6 <- eigend$vectors[, 6]
> names(weights6) <- colnames(retp)
> barplot(weights6, names.arg=names(weights6), xlab="", ylab="",
+   main="Highest Order Principal Component Loadings")
```

Principal Component Analysis of ETF Returns

Principal Component Analysis (*PCA*) is a *dimension reduction* technique, that explains the returns of a large number of correlated time series as linear combinations of a smaller number of principal component time series.

The input time series are often scaled by their standard deviations, to improve the accuracy of *PCA dimension reduction*, so that more information is retained by the first few *principal component* time series.

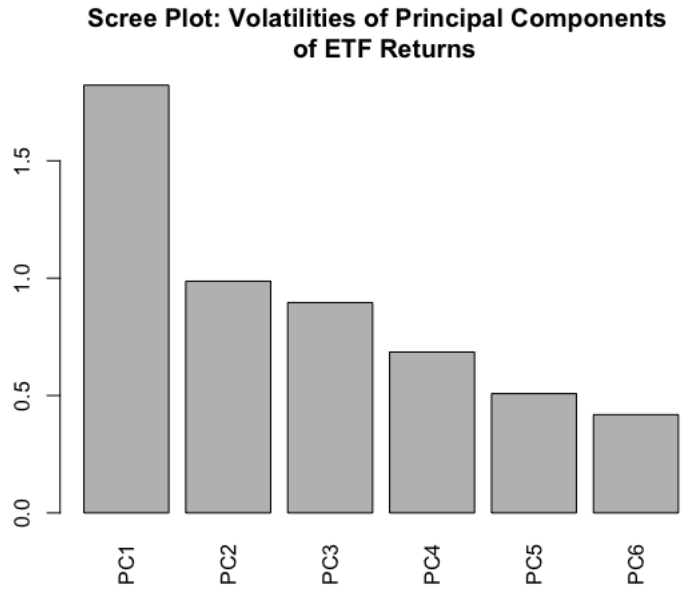
If the input time series are not scaled, then *PCA* analysis is equivalent to the *eigen decomposition* of the covariance matrix, and if they are scaled, then *PCA* analysis is equivalent to the *eigen decomposition* of the correlation matrix.

The function `prcomp()` performs *Principal Component Analysis* on a matrix of data (with the time series as columns), and returns the results as a list of class `prcomp`.

The `prcomp()` argument `scale=TRUE` specifies that the input time series should be scaled by their standard deviations.

The *Kaiser-Guttman* rule uses only *principal components* with *variance* greater than 1.

Another rule is to use the *principal components* with the largest standard deviations which sum up to 80% of the total variance of returns.



A *scree plot* is a bar plot of the volatilities of the *principal components*.

```
> # Perform principal component analysis PCA
> pcad <- prcomp(retp, scale=TRUE)
> # Plot standard deviations of principal components
> barplot(pcad$sdev, names.arg=colnames(pcad$rotation),
+   las=3, xlab="", ylab="",
+   main="Scree Plot: Volatilities of Principal Components \n of ETF
> # Calculate the number of principal components which sum up to at
> pcavar <- pcad$sdev^2
> which(cumsum(pcavar)/sum(pcavar) > 0.8)[1]
```

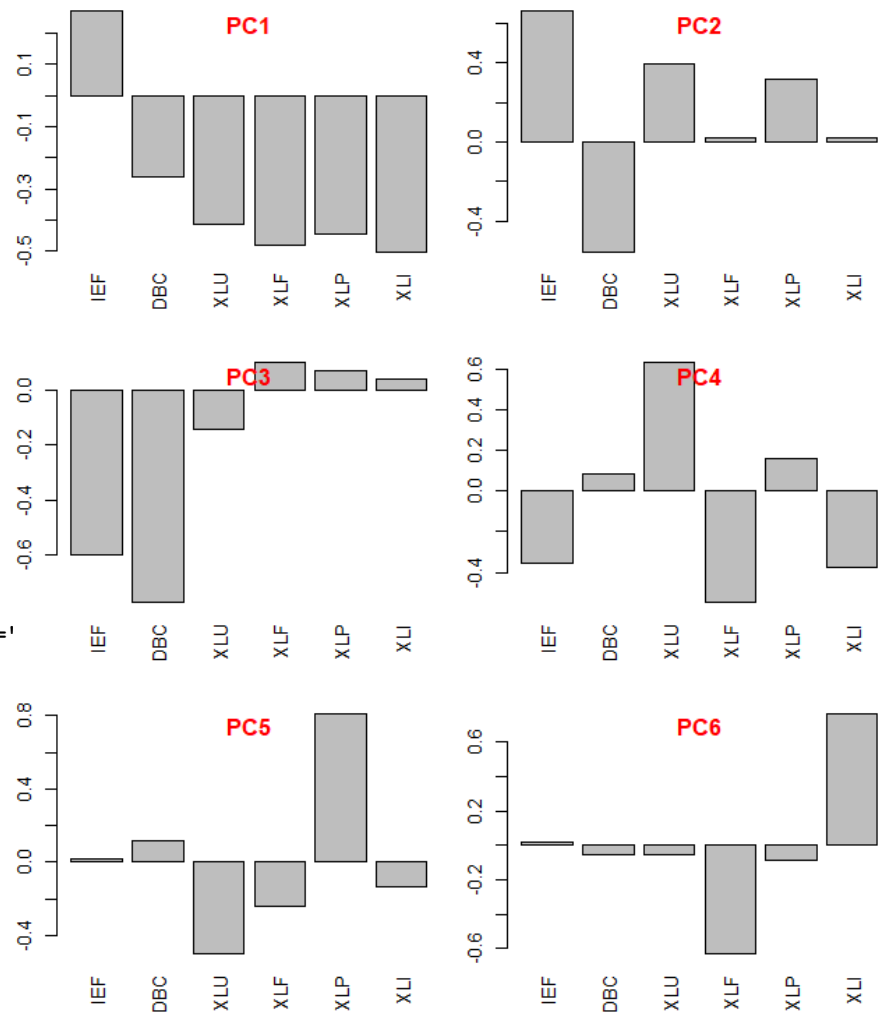
Principal Component Loadings (Weights)

Principal component loadings are the weights of portfolios which have mutually orthogonal returns.

The *principal component* (*PC*) portfolios represent the different orthogonal modes of the return variance.

The *PC* portfolios typically consist of long or short positions of highly correlated groups of assets (clusters), so that they represent relative value portfolios.

```
> # Plot barplots with PCA loadings (weights) in multiple panels
> pcad$rotation
> # x11(width=6, height=7)
> par(mfrow=c(nweights/2, 2))
> par(mar=c(3, 2, 2, 1), oma=c(0, 0, 0, 0))
> for (ordern in 1:nweights) {
+   barplot(pcad$rotation[, ordern], las=3, xlab="", ylab="", main='
+   title(paste0("PC", ordern), line=-1, col.main="red")
+ }  # end for
```



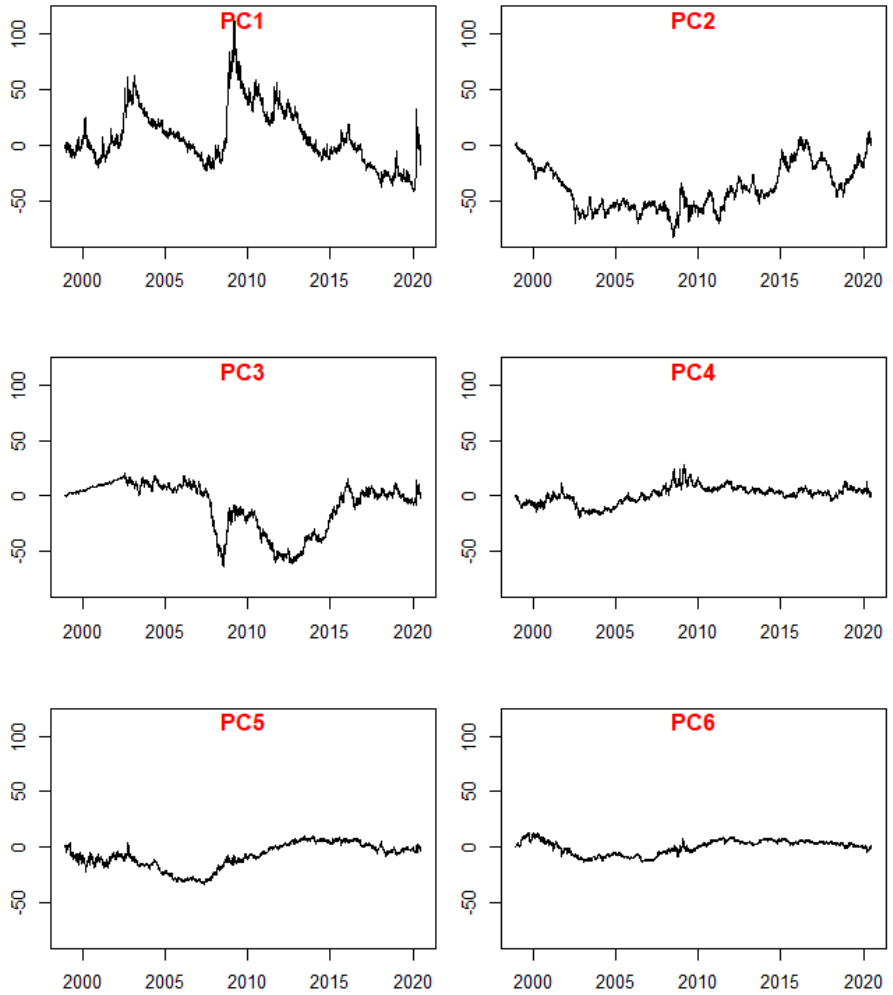
Principal Component Time Series

The time series of the *principal components* can be calculated by multiplying the loadings (weights) times the original data.

The *principal component* time series have mutually orthogonal returns.

Higher order *principal components* are gradually less volatile.

```
> # Calculate the products of principal component time series
> round(t(pcad$x) %*% pcad$x, 2)
> # Calculate the principal component time series from returns
> datev <- zoo::index(pricev)
> retpca <- xts::xts(retp %*% pcad$rotation, order.by=datev)
> round(cov(retpca), 3)
> all.equal(coredata(retpca), pcad$x, check.attributes=FALSE)
> retpcac <- cumsum(retpca)
> # Plot principal component time series in multiple panels
> rangev <- range(retpcac)
> for (ordern in 1:nweights) {
+   plot.zoo(retpcac[, ordern], ylim=rangev, xlab="", ylab="")
+   title(paste0("PC", ordern), line=-1, col.main="red")
+ }  # end for
```



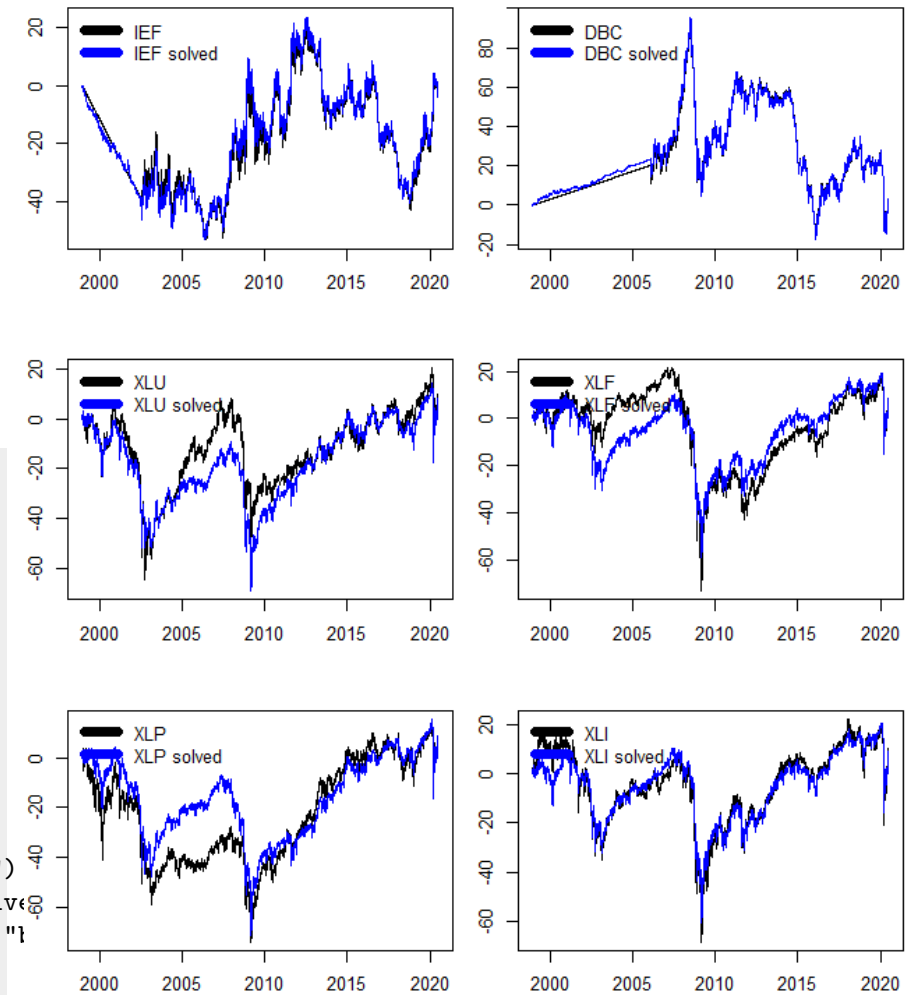
Dimension Reduction Using Principal Component Analysis

The original time series can be calculated exactly from the time series of all the *principal components*, by inverting the loadings matrix.

The original time series can be calculated approximately from just the first few *principal components*, which demonstrates that *PCA* is a form of *dimension reduction*.

The function `solve()` solves systems of linear equations, and also inverts square matrices.

```
> # Invert all the principal component time series
> retpca <- retp %*% pcad$rotation
> solved <- retpca %*% solve(pcad$rotation)
> all.equal(coredata(retp), solved)
> # Invert first 3 principal component time series
> solved <- retpca[, 1:3] %*% solve(pcad$rotation)[1:3, ]
> solved <- xts::xts(solved, datev)
> solved <- cumsum(solved)
> retc <- cumsum(retp)
> # Plot the solved returns
> for (symbol in symbolv) {
+   plot.zoo(cbind(retc[, symbol], solved[, symbol]),
+     plot.type="single", col=c("black", "blue"), xlab="", ylab="")
+   legend(x="topleft", bty="n", legend=paste0(symbol, c("", " solve
+    title=NULL, inset=0.0, cex=1.0, lwd=6, lty=1, col=c("black", "b
+ }  # end for
```



Condition Number of Correlation Matrices

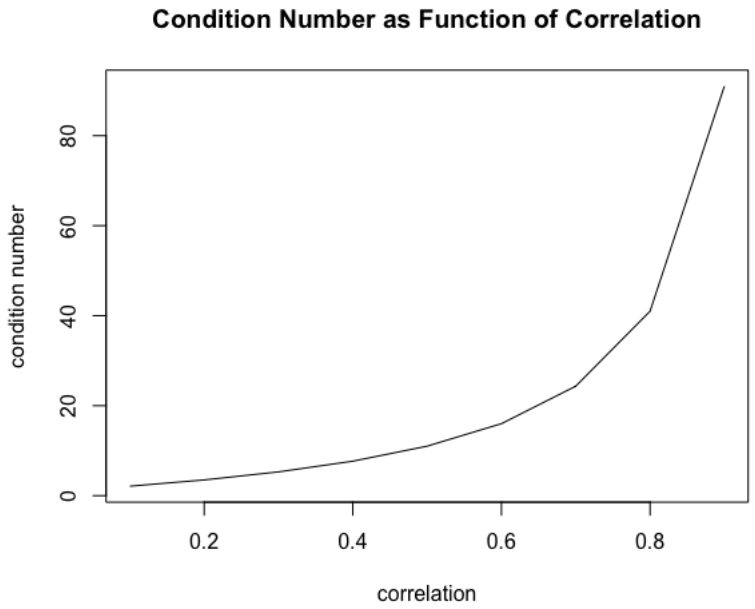
The condition number κ of a correlation matrix is equal to the ratio of its largest eigenvalue divided by the smallest:

$$\kappa = \frac{\lambda_{max}}{\lambda_{min}}$$

The condition number depends on the level of correlations. If correlations are small then the eigenvalues are close to 1 and the condition number is also close to 1. If the correlations are close to 1 then the condition number is large.

A large condition number indicates the presence of small eigenvalues, and a correlation matrix close to *singular*, with a poorly defined inverse matrix.

A very large condition number indicates that the correlation matrix is close to being *singular*.




```
> # Create a matrix with low correlation
> ndata <- 10
> cormat <- matrix(rep(0.1, ndata^2), nc=ndata)
> diag(cormat) <- rep(1, ndata)
> # Calculate the condition number
> eigend <- eigen(cormat)
> eigenval <- eigend$values
> max(eigenval)/min(eigenval)
> # Create a matrix with high correlation
> cormat <- matrix(rep(0.9, ndata^2), nc=ndata)
> diag(cormat) <- rep(1, ndata)
> # Calculate the condition number
> eigend <- eigen(cormat)
> eigenval <- eigend$values
> max(eigenval)/min(eigenval)
```

```
> # Calculate the condition numbers as function correlation
> corvec <- seq(0.1, 0.9, 0.1)
> condvec <- sapply(corvec, function(corv) {
+   cormat <- matrix(rep(corv, ndata^2), nc=ndata)
+   diag(cormat) <- rep(1, ndata)
+   eigend <- eigen(cormat)
+   eigenval <- eigend$values
+   max(eigenval)/min(eigenval)
+ })  # end sapply
> # Plot the condition numbers
> plot(x=corvec, y=condvec, t="l",
+   main="Condition Number as Function of Correlation",
+   xlab="correlation", ylab="condition number")
```

Condition Number for Small Number of Observations

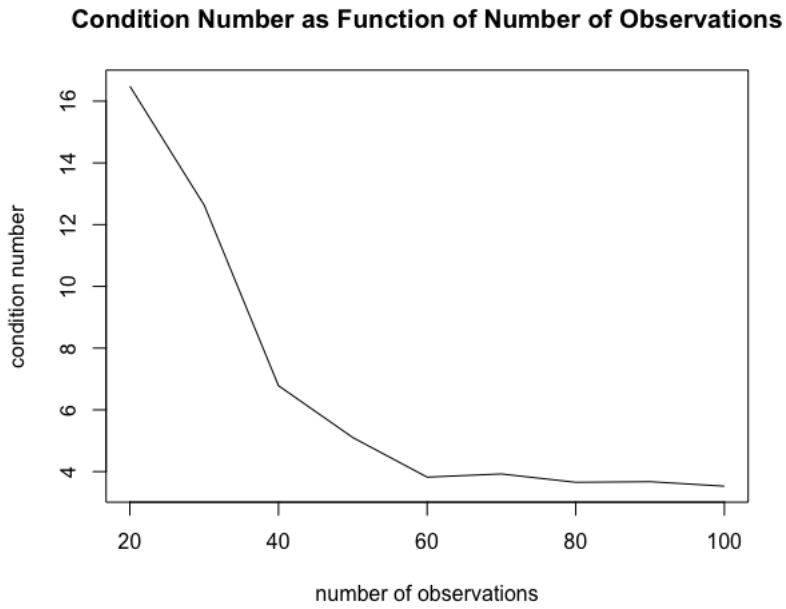
The condition number also depends on the number of observations.

If the number of observations (rows of data) is small compared to the number of stocks (columns), then the condition number can be large, even if the returns are not correlated.

That's because as the number of rows of data decreases, the returns become more *collinear*, and the sample correlation matrix becomes more *singular*, with some very small eigenvalues.

In practice, calculating the inverse correlation matrix of returns faces two challenges: not enough rows of data and correlated returns.

In both cases, the problem is that the columns of returns are close to *collinear*.




```
> # Simulate uncorrelated stock returns
> nstocks <- 10
> nrows <- 100
> # Initialize the random number generator
> set.seed(1121, "Mersenne-Twister", sample.kind="Rejection")
> retp <- matrix(rnorm(nstocks*nrows), nc=nstocks)
> # Calculate the condition numbers as function of number of observations
> obsvec <- seq(20, nrows, 10)
> condvec <- sapply(obsvec, function(nobs) {
+   cormat <- cor(retp[1:nobs, ])
+   eigend <- eigen(cormat)
+   eigenval <- eigend$values
+   max(eigenval)/min(eigenval)
+ })  # end sapply
```

```
> # Plot the condition numbers
> plot(x=obsvec, y=condvec, t="l",
+   main="Condition Number as Function of Number of Observations",
+   xlab="number of observations", ylab="condition number")
```

The Correlations of Stock Returns

Estimating the correlations of stock returns is complicated because their date ranges may not overlap in time. Stocks may trade over different date ranges because of IPOs and corporate events (takeovers, mergers).

The function `cor()` calculates the correlation matrix of time series. The argument `use="pairwise.complete.obs"` removes `NA` values from pairs of stock returns.

But removing `NA` values in pairs of stock returns can produce correlation matrices which are not positive semi-definite.

The reason is because the correlations are calculated over different time intervals for different pairs of stock returns.

```
> # Load daily S&P500 log percentage stock returns
> load(file="/Users/jerzy/Develop/lecture_slides/data/sp500_returns.
> # Calculate the number of NA values in retstock
> retp <- retstock
> colSums(is.na(retp))
> # Calculate the correlations ignoring NA values
> cor(retp$DAL, retp$FOXA, use="pairwise.complete.obs")
> cor(na.omit(retp[, c("DAL", "FOXA")]))[2]
> cormat <- cor(retp, use="pairwise.complete.obs")
> sum(is.na(cormat))
> cormat[is.na(cormat)] <- 0
```

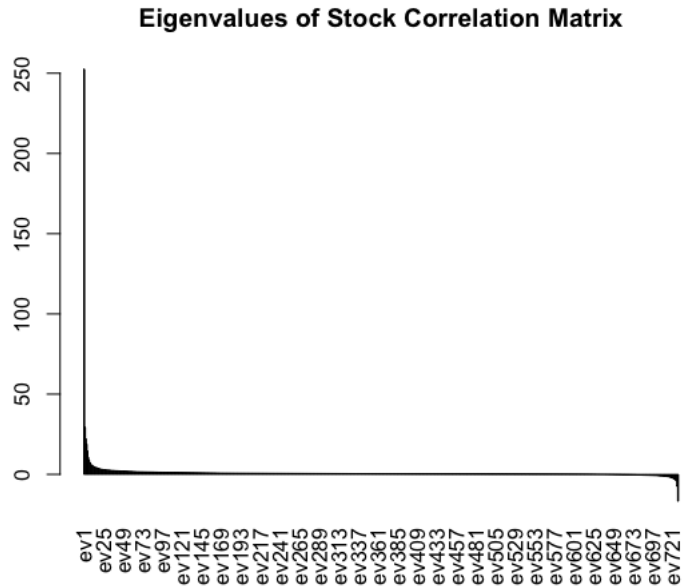
Principal Component Analysis of Stock Returns

Removing `NA` values in pairs of stock returns can produce correlation matrices which are not positive semi-definite.

The function `prcomp()` produces an error when the correlation matrix is not positive semi-definite, so instead, *eigen decomposition* can be applied to perform *Principal Component Analysis*.

If some of the eigenvalues are negative, then the condition number is calculated using the eigenvalue with the smallest absolute value.

```
> # Perform principal component analysis PCA - produces error
> pcad <- prcomp(retp, scale=TRUE)
> # Calculate the eigen decomposition of the correlation matrix
> eigend <- eigen(cormat)
> # Calculate the eigenvalues and eigenvectors
> eigenval <- eigend$values
> eigenvec <- eigend$vectors
> # Calculate the number of negative eigenvalues
> sum(eigenval<0)
> # Calculate the condition number
> max(eigenval)/min(abs(eigenval))
> # Calculate the number of eigenvalues which sum up to at least 80% of the total variance
> which(cumsum(eigenval)/sum(eigenval) > 0.8)[1]
```




```
> # Plot the eigenvalues
> barplot(eigenval, xlab="", ylab="", las=3,
+   names.arg=paste0("ev", 1:NROW(eigenval)),
+   main="Eigenvalues of Stock Correlation Matrix")
```

Principal Component Analysis of Low and High Volatility Stocks

Low and high volatility stocks have different correlations and principal components.

Low volatility stocks have higher correlations than high volatility stocks, so their correlation matrix has a larger condition number than high volatility stocks.

But low volatility stocks can be explained by a smaller number of principal components, compared to high volatility stocks.

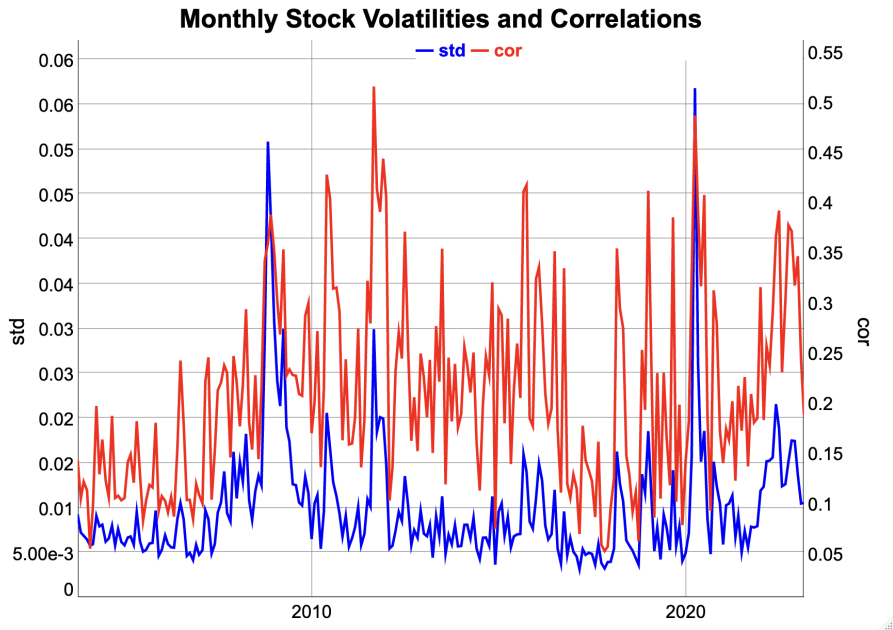
```
> # Calculate the stock variance
> varv <- sapply(retp, var, na.rm=TRUE)
> # Calculate the returns of low and high volatility stocks
> nstocks <- NCOL(retp)
> medianv <- median(varv)
> retlow <- retp[, varv <= medianv]
> rethigh <- retp[, varv > medianv]
> # Calculate the correlations of low volatility stocks
> cormat <- cor(retlow, use="pairwise.complete.obs")
> cormat[is.na(cormat)] <- 0
> # Calculate the mean correlations
> mean(cormat[upper.tri(cormat)])
> # Calculate the eigen decomposition of the correlation matrix
> eigend <- eigen(cormat)
> eigenval <- eigend$values
> # Calculate the number of negative eigenvalues
> sum(eigenval < 0)
> # Calculate the number of eigenvalues which sum up to at least 80%
> which(cumsum(eigenval)/sum(eigenval) > 0.8)[1]
> # Calculate the condition number
> max(eigenval)/min(abs(eigenval))
> # Calculate the correlations of high volatility stocks
> cormat <- cor(rethigh, use="pairwise.complete.obs")
> cormat[is.na(cormat)] <- 0
> # Calculate the mean correlations
> mean(cormat[upper.tri(cormat)])
> # Calculate the eigen decomposition of the correlation matrix
> eigend <- eigen(cormat)
> eigenval <- eigend$values
> # Calculate the number of negative eigenvalues
> sum(eigenval < 0)
> # Calculate the number of eigenvalues which sum up to at least 80%
> which(cumsum(eigenval)/sum(eigenval) > 0.8)[1]
> # Calculate the condition number
> max(eigenval)/min(abs(eigenval))
```

Stock Correlations in Periods of Low and High Volatility

Correlations of stock returns are higher in time intervals with high volatility.

Stock returns have *high correlations* in time intervals with *high volatility*, and vice versa.

```
> # Subset (select) the stock returns after the start date of VTI
> retvti <- na.omit(rutils::etfenv$returns$VTI)
> colnames(retvti) <- "VTI"
> retp <- retstock[zoo::index(retvti)]
> datev <- zoo::index(retp)
> retvti <- retvti[datev]
> nrows <- NROW(retp)
> nstocks <- NCOL(retp)
> head(retp[, 1:5])
> # Calculate the monthly end points
> endd <- rutils::calc_endpoints(retvti, interval="months")
> retvti[head(endd)]
> retvti[tail(endd)]
> # Remove stub interval at the end
> endd <- endd[-NROW(endd)]
> npts <- NROW(endd)
> # Calculate the monthly stock volatilities and correlations
> stdcor <- sapply(2:npts, function(endp) {
+   # cat("endp = ", endp, "\n")
+   retp <- retp[endd[endp-1]:endd[endp]]
+   cormat <- cor(retp, use="pairwise.complete.obs")
+   cormat[is.na(cormat)] <- 0
+   c(stdev=sd(retvti[endd[endp-1]:endd[endp]]),
+     cor=mean(cormat[upper.tri(cormat)]))
+ })  # end sapply
> stdcor <- t(stdcor)
```




```
> # Scatterplot of stock volatilities and correlations
> plot(x=stdcor[, "stdev"], y=stdcor[, "cor"],
+  xlab="volatility", ylab="correlation",
+  main="Monthly Stock Volatilities and Correlations")
> # Plot stock volatilities and correlations
> colnamev <- colnames(stdcor)
> stdcor <- xts(stdcor, zoo::index(retvti[endd]))
> dygraphs::dygraph(stdcor,
+   main="Monthly Stock Volatilities and Correlations") %>%
+   dyAxis("y", label=colnamev[1], independentTicks=TRUE) %>%
+   dyAxis("y2", label=colnamev[2], independentTicks=TRUE) %>%
+   dySeries(name=colnamev[1], axis="y", label=colnamev[1], strokeW
+   dySeries(name=colnamev[2], axis="y2", label=colnamev[2], stroke
+   dyLegend(show="always", width=300)
```

Principal Component Analysis in Periods of Low and High Volatility

Stock returns in time intervals with *high volatility* have *high correlations* and therefore require fewer eigenvalues to explain 80% of their total variance.

Stock returns in time intervals with *low volatility* have *low correlations* and therefore require more eigenvalues to explain 80% of their total variance.

```
> # Calculate the median VTI volatility
> medianv <- median(stdcor[, "stdev"])
> # Calculate the stock returns of low volatility intervals
> retlow <- lapply(2:npts, function(endp) {
+   if (stdcor[endp-1, "stdev"] <= medianv)
+     retp[endd[endp-1]:endd[endp]]
+ })  # end lapply
> retlow <- rutils::do_call(rbind, retlow)
> # Calculate the stock returns of high volatility intervals
> rethigh <- lapply(2:npts, function(endp) {
+   if (stdcor[endp-1, "stdev"] > medianv)
+     retp[endd[endp-1]:endd[endp]]
+ })  # end lapply
> rethigh <- rutils::do_call(rbind, rethigh)
```

```
> # Calculate the correlations of low volatility intervals
> cormat <- cor(retlow, use="pairwise.complete.obs")
> cormat[is.na(cormat)] <- 0
> mean(cormat[upper.tri(cormat)])
> # Calculate the eigen decomposition of the correlation matrix
> eigend <- eigen(cormat)
> eigenval <- eigend$values
> sum(eigenval < 0)
> # Calculate the number of eigenvalues which sum up to at least 80%
> which(cumsum(eigenval)/sum(eigenval) > 0.8)[1]
> # Calculate the condition number
> max(eigenval)/min(abs(eigenval))
> # Calculate the correlations of high volatility intervals
> cormat <- cor(rethigh, use="pairwise.complete.obs")
> cormat[is.na(cormat)] <- 0
> mean(cormat[upper.tri(cormat)])
> # Calculate the eigen decomposition of the correlation matrix
> eigend <- eigen(cormat)
> eigenval <- eigend$values
> sum(eigenval < 0)
> # Calculate the number of eigenvalues which sum up to at least 80%
> which(cumsum(eigenval)/sum(eigenval) > 0.8)[1]
> # Calculate the condition number
> max(eigenval)/min(abs(eigenval))
```

Trailing Correlations of Stock Returns

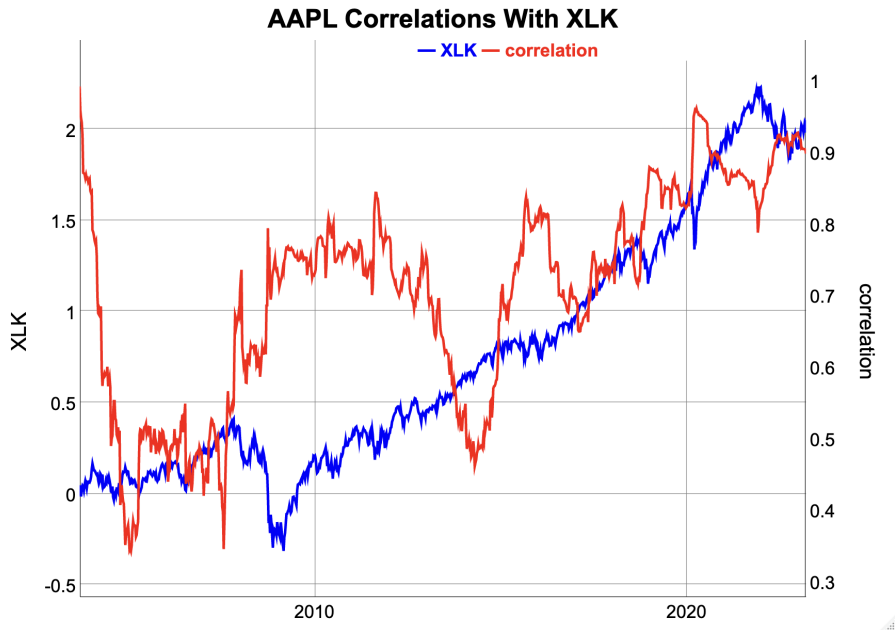
The trailing covariance can be updated using *online* recursive formulas with the weight decay factor λ:

$$\bar{x}_t = \lambda \bar{x}_{t-1} + (1-\lambda)x_t$$
$$\bar{y}_t = \lambda \bar{y}_{t-1} + (1-\lambda)y_t$$
$$\sigma^2_{xt} = \lambda \sigma^2_{x(t-1)} + (1-\lambda)(x_t - \bar{x}_t)^2$$
$$\sigma^2_{yt} = \lambda \sigma^2_{y(t-1)} + (1-\lambda)(y_t - \bar{y}_t)^2$$
$$\text{cov}_t = \lambda \, \text{cov}_{t-1} + (1-\lambda)(x_t - \bar{x}_t)(y_t - \bar{y}_t)$$

The parameter λ determines the rate of decay of the weight of past returns. If λ is close to 1 then the decay is weak and past returns have a greater weight, and the trailing mean values have a stronger dependence on past returns. This is equivalent to a long look-back interval. And vice versa if λ is close to 0.

The function `HighFreq::run_covar()` calculates the trailing variances, covariances, and means of two *time series*.

```
> # Calculate the AAPL and XLK returns
> retp <- na.omit(cbind(returns$AAPL, rutils::etfenv$returns$XLK))
> # Calculate the trailing correlations
> lambda <- 0.99
> covarv <- HighFreq::run_covar(retp, lambda)
> correlv <- covarv[, 1, drop=FALSE]/sqrt(covarv[, 2]*covarv[, 3])
```



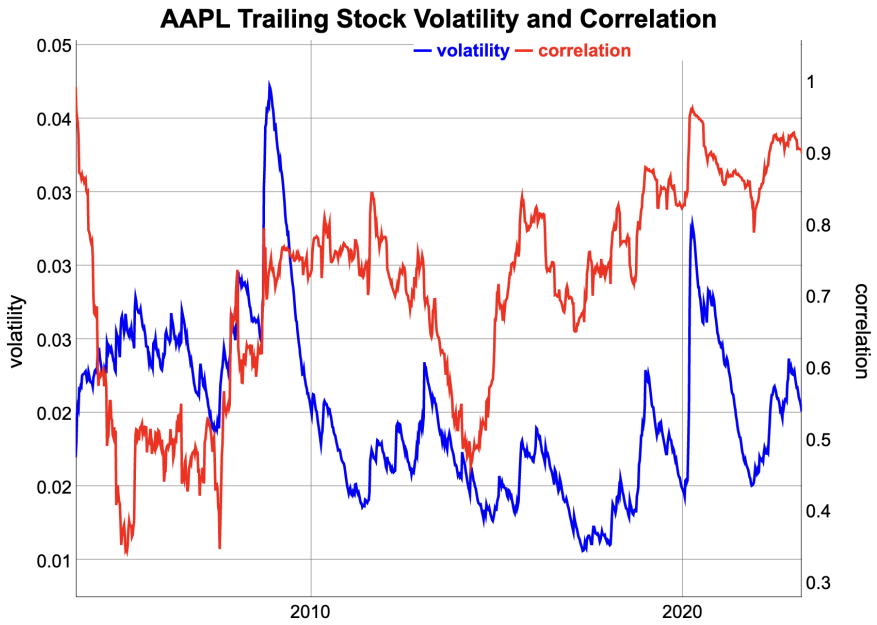

```
> # Plot dygraph of XLK returns and AAPL correlations
> datav <- cbind(cumsum(retp$XLK), correlv)
> colnames(datav)[2] <- "correlation"
> colnamev <- colnames(datav)
> endd <- rutils::calc_endpoints(retp, interval="weeks")
> dygraphs::dygraph(datav[endd], main="AAPL Correlations With XLK")
+   dyAxis("y", label=colnamev[1], independentTicks=TRUE) %>%
+   dyAxis("y2", label=colnamev[2], independentTicks=TRUE) %>%
+   dySeries(name=colnamev[1], axis="y", label=colnamev[1], strokeW
+   dySeries(name=colnamev[2], axis="y2", label=colnamev[2], stroke
+   dyLegend(show="always", width=300)
```

Trailing Stock Correlations and Volatilities

The correlations of stock returns are typically higher in periods of higher volatility, and vice versa.

But stock correlations have increased after the 2008–09 financial crisis, while volatilities have decreased.

The correlation of *AAPL* and *XLK* has increased over time because *AAPL* has become a much larger component of *XLK*, as its stock has rallied.




```
> # Scatterplot of trailing stock volatilities and correlations
> volv <- sqrt(covarv[, 2])
> plot(x=volv[endd], y=correlv[endd, ], pch=1, col="blue",
+  xlab="AAPL volatility", ylab="Correlation",
+  main="Trailing Volatilities and Correlations of AAPL vs XLK")
> # Interactive scatterplot of trailing stock volatilities and corre
> datev <- zoo::index(retp[endd])
> datav <- data.frame(datev, volv[endd], correlv[endd, ])
> colnames(datav) <- c("date", "volatility", "correlation")
> library(plotly)
> plotly::plot_ly(data=datav, x=~volatility, y=~correlation,
+   type="scatter", mode="markers", text=datev) %>%
+   layout(title="Trailing Volatilities and Correlations of AAPL vs
```

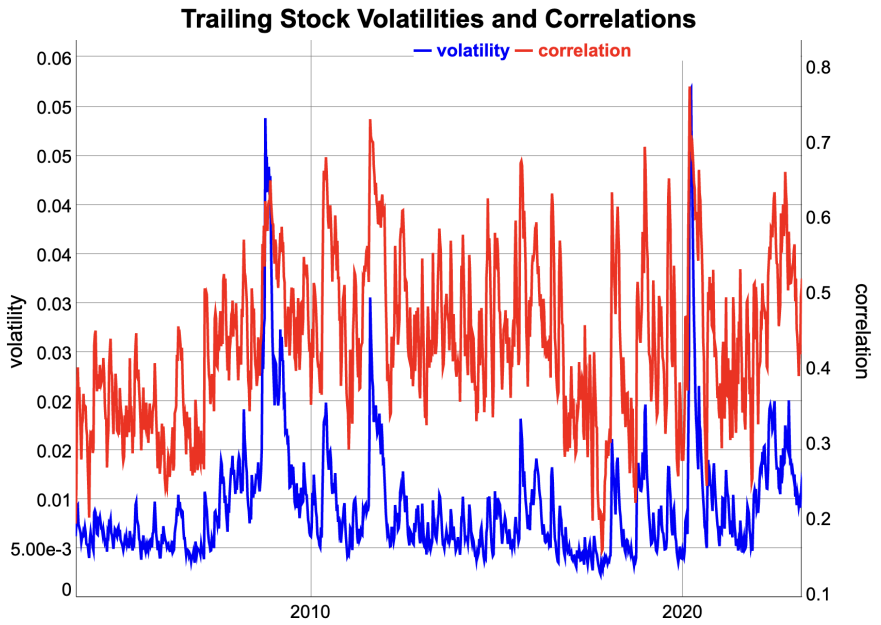
```
> # Plot trailing stock volatilities and correlations
> datav <- xts(cbind(volv, correlv), zoo::index(retp))
> colnames(datav) <- c("volatility", "correlation")
> colnamev <- colnames(datav)
> dygraphs::dygraph(datav[endd], main="AAPL Trailing Stock Volatilit
+   dyAxis("y", label=colnamev[1], independentTicks=TRUE) %>%
+   dyAxis("y2", label=colnamev[2], independentTicks=TRUE) %>%
+   dySeries(name=colnamev[1], axis="y", label=colnamev[1], strokeW
+   dySeries(name=colnamev[2], axis="y2", label=colnamev[2], stroke
+   dyLegend(show="always", width=300)
```

Stock Portfolio Correlations and Volatilities

The average correlations of a stock portfolio are typically higher in periods of higher volatility, and vice versa.

But stock correlations have increased after the 2008-09 financial crisis, while volatilities have decreased.

```
> # Calculate the portfolio returns
> retvti <- na.omit(rutils::etfenv$returns$VTI)
> colnames(retvti) <- "VTI"
> datev <- zoo::index(retvti)
> retp <- retstock100
> retp[is.na(retp)] <- 0
> retp <- retp[datev]
> nrows <- NROW(retp)
> nstocks <- NCOL(retp)
> head(retp[, 1:5])
> # Calculate the average trailing portfolio correlations
> lambda <- 0.9
> correlv <- sapply(retp, function(retp) {
+   covarv <- HighFreq::run_covar(cbind(retvti, retp), lambda)
+   covarv[, 1, drop=FALSE]/sqrt(covarv[, 2]*covarv[, 3])
+ })  # end sapply
> correlv[is.na(correlv)] <- 0
> correlp <- rowMeans(correlv)
> # Scatterplot of trailing stock volatilities and correlations
> volvti <- sqrt(HighFreq::run_var(retvti, lambda))
> endd <- rutils::calc_endpoints(retvti, interval="weeks")
> plot(x=volvti[endd], y=correlp[endd],
+  xlab="volatility", ylab="correlation",
+  main="Trailing Stock Volatilities and Correlations")
```




```
> # Plot trailing stock volatilities and correlations
> datav <- xts(cbind(volvti, correlp), datev)
> colnames(datav) <- c("volatility", "correlation")
> colnamev <- colnames(datav)
> dygraphs::dygraph(datav[endd],
+   main="Trailing Stock Volatilities and Correlations") %>%
+   dyAxis("y", label=colnamev[1], independentTicks=TRUE) %>%
+   dyAxis("y2", label=colnamev[2], independentTicks=TRUE) %>%
+   dySeries(name=colnamev[1], axis="y", label=colnamev[1], strokeW
+   dySeries(name=colnamev[2], axis="y2", label=colnamev[2], stroke
+   dyLegend(show="always", width=300)
```

Vector and Matrix Calculus

Let $\mathbf{v}$ and $\mathbf{w}$ be vectors, with $\mathbf{v} = \{v_i\}_{i=1}^{i=n}$, and let $\mathbb{1}$ be the unit vector, with $\mathbb{1} = \{1\}_{i=1}^{i=n}$.

Then the inner product of $\mathbf{v}$ and $\mathbf{w}$ can be written as $\mathbf{v}^T\mathbf{w} = \mathbf{w}^T\mathbf{v} = \sum_{i=1}^{n} v_i w_i$.

We can then express the sum of the elements of $\mathbf{v}$ as the inner product: $\mathbf{v}^T\mathbb{1} = \mathbb{1}^T\mathbf{v} = \sum_{i=1}^{n} v_i$.

And the sum of squares of $\mathbf{v}$ as the inner product: $\mathbf{v}^T\mathbf{v} = \sum_{i=1}^{n} v_i^2$.

Let $\mathbb{A}$ be a matrix, with $\mathbb{A} = \{A_{ij}\}_{i,j=1}^{i,j=n}$.

Then the inner product of matrix $\mathbb{A}$ with vectors $\mathbf{v}$ and $\mathbf{w}$ can be written as:

$$\mathbf{v}^T\mathbb{A}\,\mathbf{w} = \mathbf{w}^T\mathbb{A}^T\mathbf{v} = \sum_{i,j=1}^{n} A_{ij} v_i w_j$$

The derivative of a scalar variable with respect to a vector variable is a vector, for example:

$$\frac{d(\mathbf{v}^T\mathbb{1})}{d\mathbf{v}} = d_v[\mathbf{v}^T\mathbb{1}] = d_v[\mathbb{1}^T\mathbf{v}] = \mathbb{1}^T$$

$$d_v[\mathbf{v}^T\mathbf{w}] = d_v[\mathbf{w}^T\mathbf{v}] = \mathbf{w}^T$$

$$d_v[\mathbf{v}^T\mathbb{A}\,\mathbf{w}] = \mathbf{w}^T\mathbb{A}^T$$

$$d_v[\mathbf{v}^T\mathbb{A}\,\mathbf{v}] = \mathbf{v}^T\mathbb{A} + \mathbf{v}^T\mathbb{A}^T$$

Formula Objects

Formulas in `R` are defined using the "`~`" operator followed by a series of terms separated by the `"+"` operator.

Formulas can be defined as separate objects, manipulated, and passed to functions.

The formula "`z ~ x`" means the *response vector* z is explained by the *predictor* x (also called the *explanatory variable* or *independent variable*).

The formula "`z ~ x + y`" represents a linear model: `z = ax + by + c`.

The formula "`z ~ x - 1`" or "`z ~ x + 0`" represents a linear model with zero intercept: $z = ax$.

The function `update()` modifies existing `formulas`.

The `"."` symbol represents either all the remaining data, or the variable that was in this part of the formula.

```
> # Formula of linear model with zero intercept
> formulav <- z ~ x + y - 1
> formulav
>
> # Collapse vector of strings into single text string
> paste0("x", 1:5)
> paste(paste0("x", 1:5), collapse="+")
>
> # Create formula from text string
> formulav <- as.formula(
+   # Coerce text strings to formula
+   paste("z ~ ",
+   paste(paste0("x", 1:5), collapse="+")
+   )  # end paste
+ )  # end as.formula
> class(formulav)
> formulav
> # Modify the formula using "update"
> update(formulav, log(.) ~ . + beta)
```

Simple *Linear Regression*

A Simple Linear Regression is a linear model between a *response vector* y and a single *predictor* x, defined by the formula:

$$y_i = \alpha + \beta x_i + \varepsilon_i$$

α and β are the unknown *regression coefficients*.

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

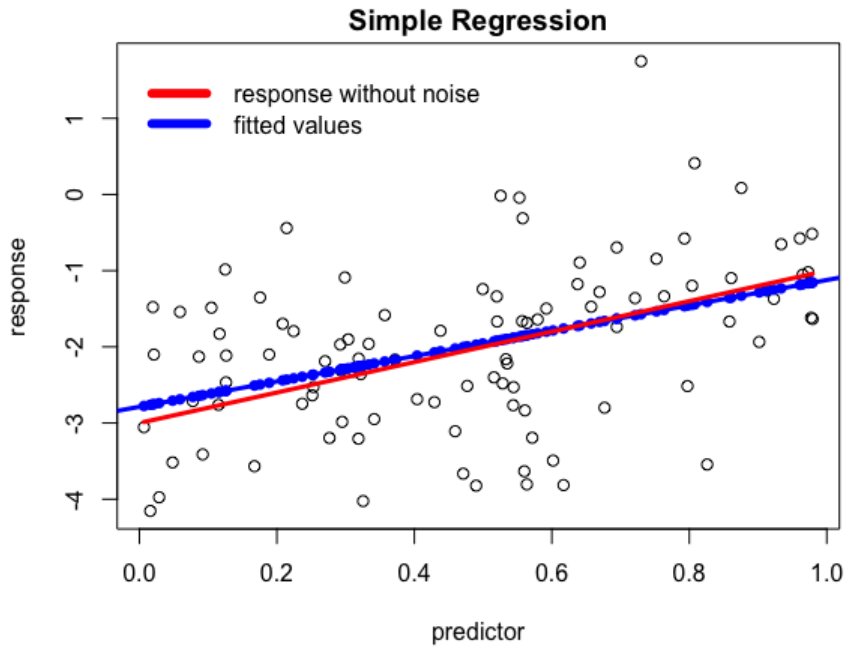
In the Ordinary Least Squares method (*OLS*), the regression parameters are estimated by minimizing the *Residual Sum of Squares* (*RSS*):

$$RSS = \sum_{i=1}^{n} \varepsilon_i^2 = \sum_{i=1}^{n} (y_i - \alpha - \beta x_i)^2$$

$$= (y - \alpha \mathbb{1} - \beta x)^T (y - \alpha \mathbb{1} - \beta x)$$

Where $\mathbb{1}$ is the unit vector, with $\mathbb{1}^T \mathbb{1} = n$ and $\mathbb{1}^T x = x^T \mathbb{1} = \sum_{i=1}^{n} x_i$

The data consists of n pairs of observations (x_i, y_i) of the response and predictor variables, with the index i ranging from 1 to n.




```
> # Define explanatory (predm) variable
> nrows <- 100
> # Initialize the random number generator
> set.seed(1121, "Mersenne-Twister", sample.kind="Rejection")
> predm <- runif(nrows)
> noisev <- rnorm(nrows)
> # Response equals linear form plus random noise
> respv <- (-3 + 2*predm + noisev)
```

The *response vector* and the *predictor matrix* don't have to be normally distributed.

Solution of *Linear Regression*

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

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

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

The solution for α is given by:

$$\alpha = \bar{y} - \beta\bar{x}$$

The solution for β can be obtained by manipulating the equation for RSS_β as follows:

$$(y - (\bar{y} - \beta\bar{x})\mathbb{1} - \beta x)^T(x - \bar{x}\mathbb{1}) =$$

$$((y - \bar{y}\mathbb{1}) - \beta(x - \bar{x}\mathbb{1}))^T(x - \bar{x}\mathbb{1}) =$$

$$(\hat{y} - \beta\hat{x})^T\hat{x} = \hat{y}^T\hat{x} - \beta\hat{x}^T\hat{x} = 0$$

Where $\hat{x} = x - \bar{x}\mathbb{1}$ and $\hat{y} = y - \bar{y}\mathbb{1}$ are the centered (de-meaned) variables. Then β is given by:

$$\beta = \frac{\hat{y}^T\hat{x}}{\hat{x}^T\hat{x}} = \frac{\sigma_y}{\sigma_x}\rho_{xy}$$

β is proportional to the correlation coefficient ρ_{xy} between the response and predictor variables.

If the response and predictor variables have zero mean, then $\alpha = 0$ and $\beta = \frac{y^T x}{x^T x}$.

The *residuals* $\varepsilon = y - \alpha\mathbb{1} - \beta x$ have zero mean: $RSS_\alpha = -2\varepsilon^T\mathbb{1} = 0$.

The *residuals* ε are orthogonal to the *predictor* x: $RSS_\beta = -2\varepsilon^T x = 0$.

The expected value of the *RSS* is equal to the *degrees of freedom* $(n-2)$ times the variance σ_ε^2 of the *residuals* ε_i: $\mathbb{E}[RSS] = (n-2)\sigma_\varepsilon^2$.

```
> # Calculate the regression beta
> betac <- cov(predm, respv)/var(predm)
> # Calculate the regression alpha
> alphac <- mean(respv) - betac*mean(predm)
```

Linear Regression Using Function `lm()`

Let the data generating process for the response variable be given as: $z = \alpha_{lat} + \beta_{lat} x + \varepsilon_{lat}$

Where α_{lat} and β_{lat} are latent (unknown) coefficients, and ε_{lat} is an unknown vector of random noise (error terms).

The error terms are the difference between the measured values of the response minus the (unknown) actual response values.

The function `lm()` fits a linear model into a set of data, and returns an object of class `"lm"`, which is a list containing the results of fitting the model:

- call - the model formula,
- coefficients - the fitted model coefficients (α, β_j),
- residuals - the model residuals (respv minus fitted values),

The regression *residuals* are not the same as the error terms, because the regression coefficients are not equal to the coefficients of the data generating process.

```
> # Specify regression formula
> formulav <- respv ~ predm
> regmod <- lm(formulav)  # Perform regression
> class(regmod)  # Regressions have class lm
[1] "lm"
> attributes(regmod)
$names
 [1] "coefficients"  "residuals"     "effects"       "rank"
 [5] "fitted.values" "assign"        "qr"            "df.residual"
 [9] "xlevels"       "call"          "terms"         "model"

$class
[1] "lm"
> eval(regmod$call$formula)  # Regression formula
respv ~ predm
> regmod$coeff  # Regression coefficients
(Intercept)       predm
      -2.79        1.67
> all.equal(coef(regmod), c(alphac, betac),
+       check.attributes=FALSE)
[1] TRUE
```

The *Fitted Values* of Linear Regression

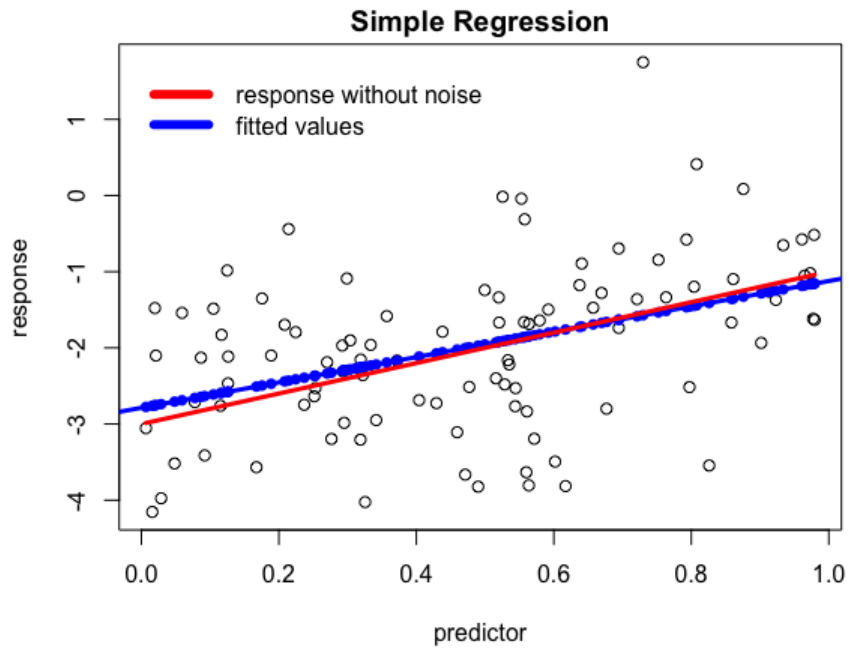
The *fitted values* y_{fit} are the estimates of the *response vector* obtained from the regression model:

$$y_{fit} = \alpha + \beta x$$

The *generic function* `plot()` produces a scatterplot when it's called on the regression formula.

`abline()` plots a straight line corresponding to the regression coefficients, when it's called on the regression object.

```
> fitv <- (alphac + betac*predm)
> all.equal(fitv, regmod$fitted.values, check.attributes=FALSE)
> # Plot scatterplot using formula
> plot(formulav, xlab="predictor", ylab="response")
> title(main="Simple Regression", line=0.5)
> # Add regression line
> abline(regmod, lwd=3, col="blue")
> # Plot fitted (forecast) response values
> points(x=predm, y=regmod$fitted.values, pch=16, col="blue")
```



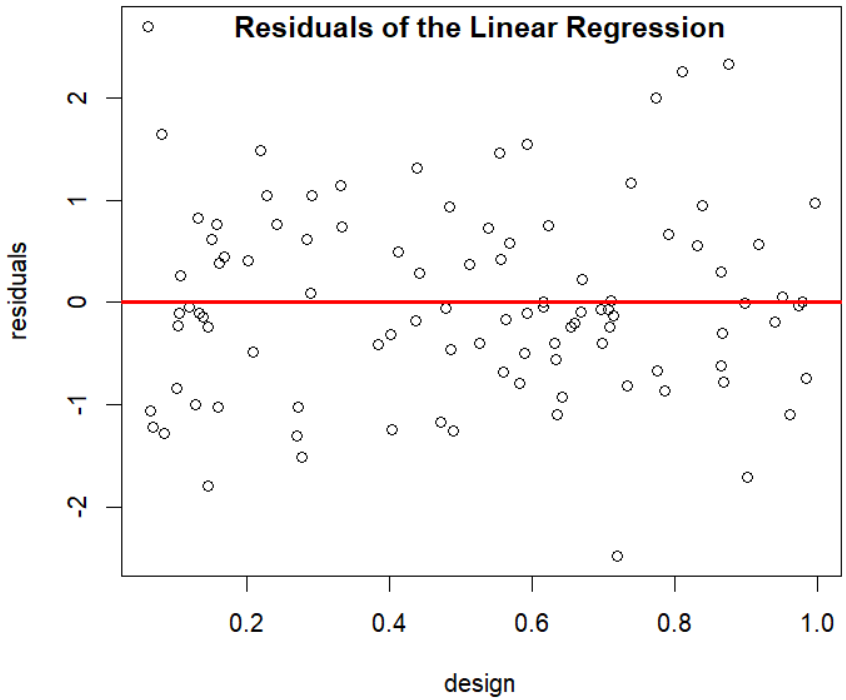

```
> # Plot response without noise
> lines(x=predm, y=(respv-noisev), col="red", lwd=3)
> legend(x="topleft", # Add legend
+        legend=c("response without noise", "fitted values"),
+        title=NULL, inset=0.0, cex=1.0, y.intersp=0.3,
+        bty="n", lwd=6, lty=1, col=c("red", "blue"))
```

Linear Regression Residuals

The *residuals* ε_i of a *linear regression* are defined as the *response vector* minus the fitted values:

$$\varepsilon_i = y_i - y_{fit}$$

```
> # Calculate the residuals
> fitv <- (alphac + betac*predm)
> resids <- (respv - fitv)
> all.equal(resids, regmod$residuals, check.attributes=FALSE)
[1] TRUE
> # Residuals are orthogonal to the predictor
> all.equal(sum(resids*predm), target=0)
[1] TRUE
> # Residuals are orthogonal to the fitted values
> all.equal(sum(resids*fitv), target=0)
[1] TRUE
> # Sum of residuals is equal to zero
> all.equal(mean(resids), target=0)
[1] TRUE
```




```
> x11(width=6, height=5)  # Open x11 for plotting
> # Set plot parameters to reduce whitespace around plot
> par(mar=c(5, 5, 1, 1), oma=c(0, 0, 0, 0))
> # Extract residuals
> datav <- cbind(predm, regmod$residuals)
> colnames(datav) <- c("predictor", "residuals")
> # Plot residuals
> plot(datav)
> title(main="Residuals of the Linear Regression", line=-1)
> abline(h=0, lwd=3, col="red")
```

Standard Errors of Regression Coefficients

The *residuals* are the source of error in the regression model, producing uncertainty in the *response vector y* and in the regression coefficients: $y_i = \alpha + \beta x_i + \varepsilon_i$.

The standard errors of the regression coefficients are equal to their standard deviations, given the *residuals* as the source of error.

Since $\beta = \frac{\hat{y}^T \hat{x}}{\hat{x}^T \hat{x}}$, then its variance is equal to:

$$\sigma_\beta^2 = \frac{1}{(n-2)} \frac{E[(\varepsilon^T \hat{x})^2]}{(\hat{x}^T \hat{x})^2} = \frac{1}{(n-2)} \frac{E[\varepsilon^2]}{\hat{x}^T \hat{x}} = \frac{\sigma_\varepsilon^2}{\hat{x}^T \hat{x}}$$

Since $\alpha = \bar{y} - \beta \bar{x}$, then its variance is equal to:

$$\sigma_\alpha^2 = \frac{\sigma_\varepsilon^2}{n} + \sigma_\beta^2 \bar{x}^2 = \sigma_\varepsilon^2 (\frac{1}{n} + \frac{\bar{x}^2}{\hat{x}^T \hat{x}})$$

```
> # Calculate the centered (de-meaned) predictor and response vecto
> predc <- predm - mean(predm)
> respc <- respv - mean(respv)
> # Degrees of freedom of residuals
> degf <- regmod$df.residual
> # Standard deviation of residuals
> residsd <- sqrt(sum(resids^2)/degf)
> # Standard error of beta
> betasd <- residsd/sqrt(sum(predc^2))
> # Standard error of alpha
> alphasd <- residsd*sqrt(1/nrows + mean(predm)^2/sum(predc^2))
```

Linear Regression Summary

The function `summary.lm()` produces a list of regression model diagnostic statistics:

- coefficients: matrix with estimated coefficients, their t-statistics, and p-values,
- r.squared: fraction of response variance explained by the model,
- adj.r.squared: r.squared adjusted for higher model complexity,
- fstatistic: ratio of variance explained by the model divided by unexplained variance,

The regression `summary` is a list, and its elements can be accessed individually.

```
> regsum <- summary(regmod)  # Copy regression summary
> regsum  # Print the summary to console

Call:
lm(formula = formulav)

Residuals:
   Min     1Q Median     3Q    Max
-2.133 -0.649  0.106  0.590  3.321

Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept)   -2.787      0.196  -14.20  < 2e-16 ***
predm          1.665      0.357    4.67  9.8e-06 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 0.988 on 98 degrees of freedom
Multiple R-squared:  0.182,Adjusted R-squared:  0.173
F-statistic: 21.8 on 1 and 98 DF,  p-value: 9.75e-06
> attributes(regsum)$names  # get summary elements
 [1] "call"          "terms"         "residuals"     "coefficients"
 [5] "aliased"       "sigma"         "df"            "r.squared"
 [9] "adj.r.squared" "fstatistic"    "cov.unscaled"
```

Regression Model Diagnostic Statistics

The *null hypothesis* for regression is that the coefficients are *zero*.

The *t*-statistic (*t*-value) is the ratio of the estimated value divided by its standard error.

The *p*-value is the probability of obtaining values exceeding the *t*-statistic, assuming the *null hypothesis* is true.

A small *p*-value means that the regression coefficients are very unlikely to be zero (given the data).

The key assumption in the formula for the standard error is that the *residuals* are normally distributed, independent, and stationary.

If they are not, then the standard error and the *p*-value may be much bigger than reported by `summary.lm()`, and therefore the regression may not be statistically significant.

Asset returns are very far from normal, so the small *p*-values shouldn't be automatically interpreted as meaning that the regression is statistically significant.

```
> regsum$coeff
            Estimate Std. Error t value Pr(>|t|)
(Intercept)    -2.79      0.196  -14.20 1.61e-25
predm           1.67      0.357    4.67 9.75e-06
> # Standard errors
> regsum$coefficients[2, "Std. Error"]
[1] 0.357
> all.equal(c(alphasd, betasd), regsum$coefficients[, "Std. Error"],
+   check.attributes=FALSE)
[1] TRUE
> # R-squared
> regsum$r.squared
[1] 0.182
> regsum$adj.r.squared
[1] 0.173
> # F-statistic and ANOVA
> regsum$fstatistic
value numdf dendf
 21.8   1.0  98.0
> anova(regmod)
Analysis of Variance Table

Response: respv
          Df Sum Sq Mean Sq F value  Pr(>F)
predm      1   21.3   21.25    21.8 9.8e-06 ***
Residuals 98   95.7    0.98
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

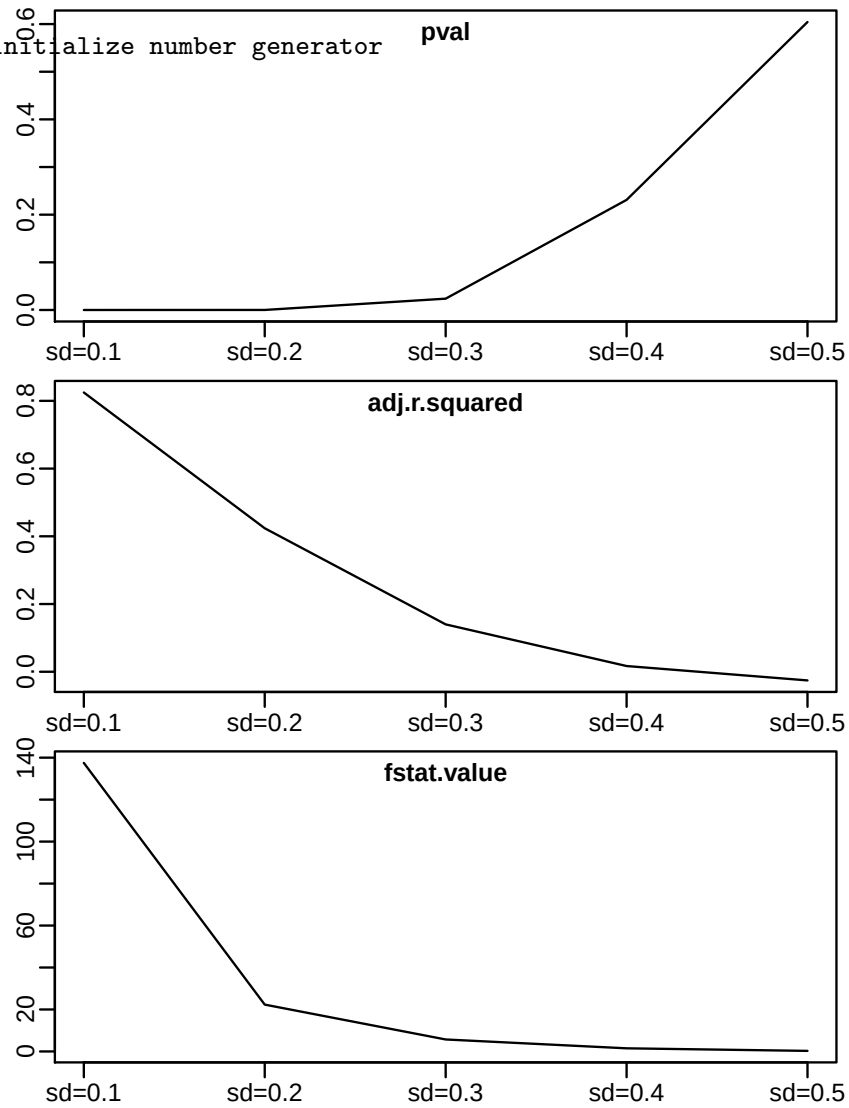
Weak Regression

If the relationship between the response and predictor variables is weak compared to the error terms (noisev), then the regression will have low statistical significance.

```
> set.seed(1121, "Mersenne-Twister", sample.kind="Rejection")
> # High noise compared to coefficient
> respv <- (-3 + 2*predm + rnorm(nrows, sd=8))
> regmod <- lm(formulav)  # Perform regression
> # Values of regression coefficients are not
> # Statistically significant
> summary(regmod)

Call:
lm(formula = formulav)

Residuals:
    Min      1Q  Median      3Q     Max
-16.430  -4.325   0.735   4.365  16.720

Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept)    -1.65       1.44   -1.14     0.26
predm          -1.70       2.62   -0.65     0.52

Residual standard error: 7.25 on 98 degrees of freedom
Multiple R-squared:  0.0043,Adjusted R-squared:  -0.00586
F-statistic: 0.423 on 1 and 98 DF,  p-value: 0.517
```

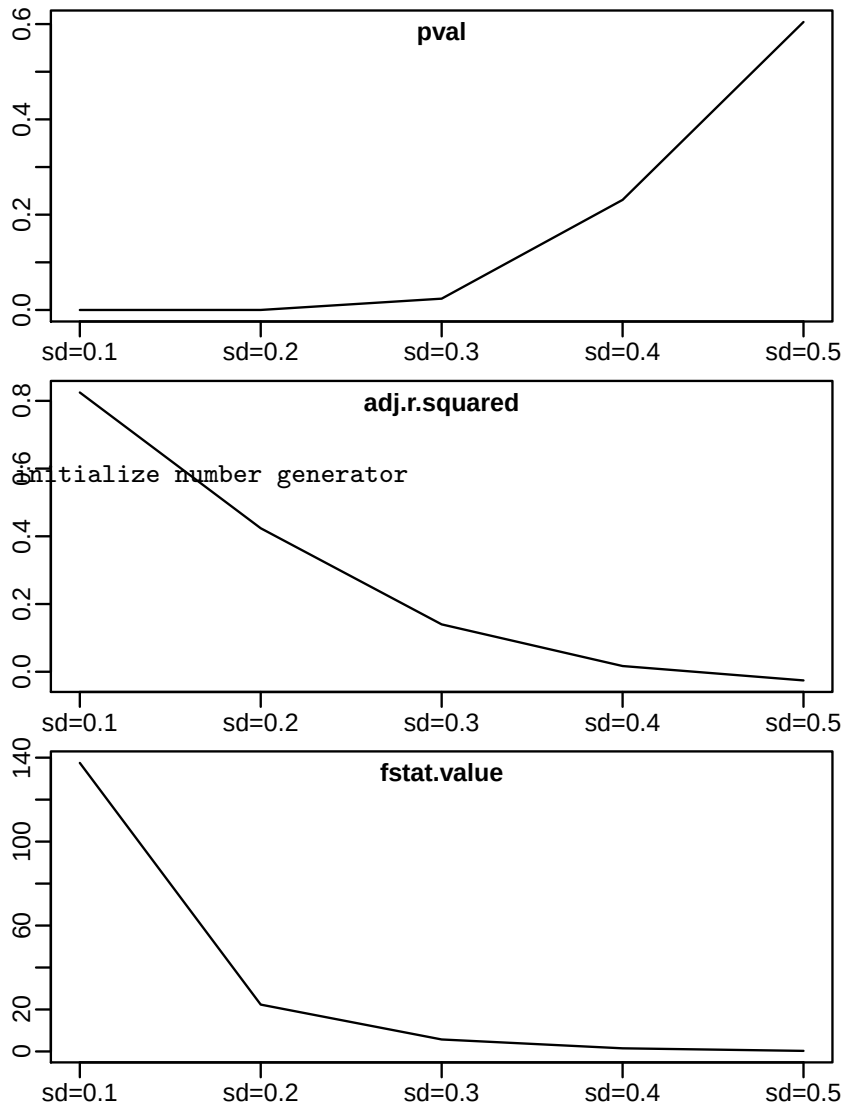
Influence of Noise on Regression

```
> regstats <- function(stdev) {  # Noisy regression
+   set.seed(1121, "Mersenne-Twister", sample.kind="Rejection")  # initialize number generator
+ # Define explanatory (predm) and response variables
+   predm <- rnorm(100, mean=2)
+   respv <- (1 + 0.2*predm + rnorm(nrows, sd=stdev))
+ # Specify regression formula
+   formulav <- respv ~ predm
+ # Perform regression and get summary
+   regsum <- summary(lm(formulav))
+ # Extract regression statistics
+   with(regsum, c(pval=coefficients[2, 4],
+    adj_rsquared=adj.r.squared,
+    fstat=fstatistic[1]))
+ }  # end regstats
> # Apply regstats() to vector of stdev dev values
> vecsd <- seq(from=0.1, to=0.5, by=0.1)
> names(vecsd) <- paste0("sd=", vecsd)
> statsmat <- t(sapply(vecsd, regstats))
> # Plot in loop
> par(mfrow=c(NCOL(statsmat), 1))
> for (it in 1:NCOL(statsmat)) {
+   plot(statsmat[, it], type="l",
+  xaxt="n", xlab="", ylab="", main="")
+   title(main=colnames(statsmat)[it], line=-1.0)
+   axis(1, at=1:(NROW(statsmat)), labels=rownames(statsmat))
+ }  # end for
```



Influence of Noise on Regression Another Method

```
> regstats <- function(datav) {  # get regression
+ # Perform regression and get summary
+   colnamev <- colnames(datav)
+   formulav <- paste(colnamev[2], colnamev[1], sep="~")
+   regsum <- summary(lm(formulav, data=datav))
+ # Extract regression statistics
+   with(regsum, c(pval=coefficients[2, 4],
+    adj_rsquared=adj.r.squared,
+    fstat=fstatistic[1]))
+ }  # end regstats
> # Apply regstats() to vector of stdev dev values
> vecsd <- seq(from=0.1, to=0.5, by=0.1)
> names(vecsd) <- paste0("sd=", vecsd)
> statsmat <- t(sapply(vecsd, function(stdev) {
+     set.seed(1121, "Mersenne-Twister", sample.kind="Rejection")  # initialize number generator
+ # Define explanatory (predm) and response variables
+     predm <- rnorm(100, mean=2)
+     respv <- (1 + 0.2*predm + rnorm(nrows, sd=stdev))
+     regstats(data.frame(predm, respv))
+     }))
> # Plot in loop
> par(mfrow=c(NCOL(statsmat), 1))
> for (it in 1:NCOL(statsmat)) {
+   plot(statsmat[, it], type="l",
+  xaxt="n", xlab="", ylab="", main="")
+   title(main=colnames(statsmat)[it], line=-1.0)
+   axis(1, at=1:(NROW(statsmat)),
+  labels=rownames(statsmat))
+ }  # end for
```



Linear Regression Diagnostic Plots

`plot()` produces diagnostic scatterplots for the *residuals*, when called on the regression object.

The diagnostic scatterplots allow for visual inspection to determine the quality of the regression fit.

"Residuals vs Fitted" is a scatterplot of the residuals vs. the forecast responses.

"Scale-Location" is a scatterplot of the square root of the standardized residuals vs. the forecast responses.

The residuals should be randomly distributed around the horizontal line representing zero residual error.

A pattern in the residuals indicates that the model was not able to capture the relationship between the variables, or that the variables don't follow the statistical assumptions of the regression model.

"Normal Q-Q" is the standard Q-Q plot, and the points should fall on the diagonal line, indicating that the residuals are normally distributed.

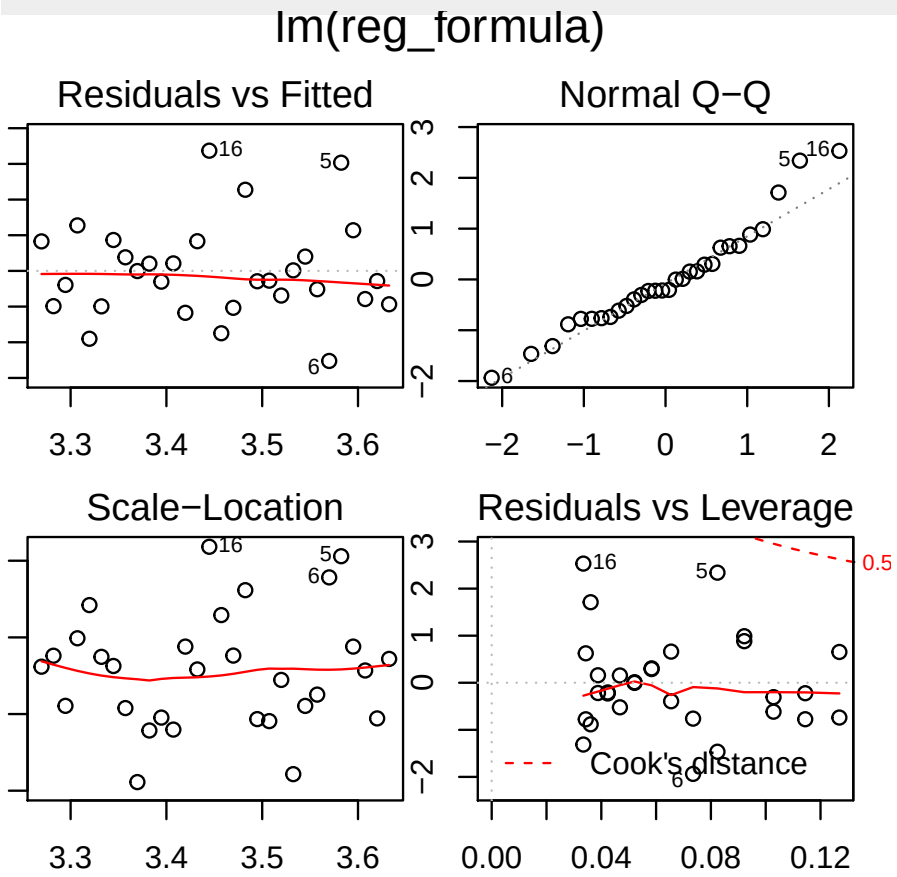
"Residuals vs Leverage" is a scatterplot of the residuals vs. their leverage.

Leverage measures the amount by which the fitted values would change if the response values were shifted by a small amount.

Cook's distance measures the influence of a single observation on the fitted values, and is proportional to the sum of the squared differences between forecasts made with all observations and forecasts made without the observation.

Points with large leverage, or a Cook's distance greater than 1 suggest the presence of an outlier or a poor model,

```
> par(mfrow=c(2, 2))  # Plot 2x2 panels
> plot(regmod)  # Plot diagnostic scatterplots
> plot(regmod, which=2)  # Plot just Q-Q
```



Durbin-Watson Test of Autocorrelation of Residuals

The *Durbin-Watson* test is designed to test the *null hypothesis* that the autocorrelations of regression *residuals* are equal to zero.

The test statistic is equal to:

$$DW = \frac{\sum_{i=2}^{n}(\varepsilon_i - \varepsilon_{i-1})^2}{\sum_{i=1}^{n}\varepsilon_i^2}$$

Where ε_i are the regression *residuals*.

The value of the *Durbin-Watson* statistic *DW* is close to zero for large positive autocorrelations, and close to four for large negative autocorrelations.

The *DW* is close to two for autocorrelations close to zero.

The *p*-value for the `reg_model` regression is large, and we conclude that the *null hypothesis* is `TRUE`, and the regression *residuals* are uncorrelated.

```
> library(lmtest)  # Load lmtest
> # Perform Durbin-Watson test
> lmtest::dwtest(regmod)

Durbin-Watson test

data:  regmod
DW = 2, p-value = 0.7
alternative hypothesis: true autocorrelation is greater than 0
```

draft: Autocorrelated Time Series Regression

Filtering or smoothing a time series containing an error terms over overlapping periods introduces autocorrelations in the error terms of the time series.

Autocorrelations in the error terms introduces autocorrelations of the regression residuals, causing the Durbin-Watson test to fail.

Autocorrelations in the error terms introduce autocorrelations of the regression residuals, causing the Durbin-Watson test to fail.

The failure of the Durbin-Watson test means that the *standard errors* and *p*-values calculated by the regression model are too small, and therefore the regression may not be statistically significant.

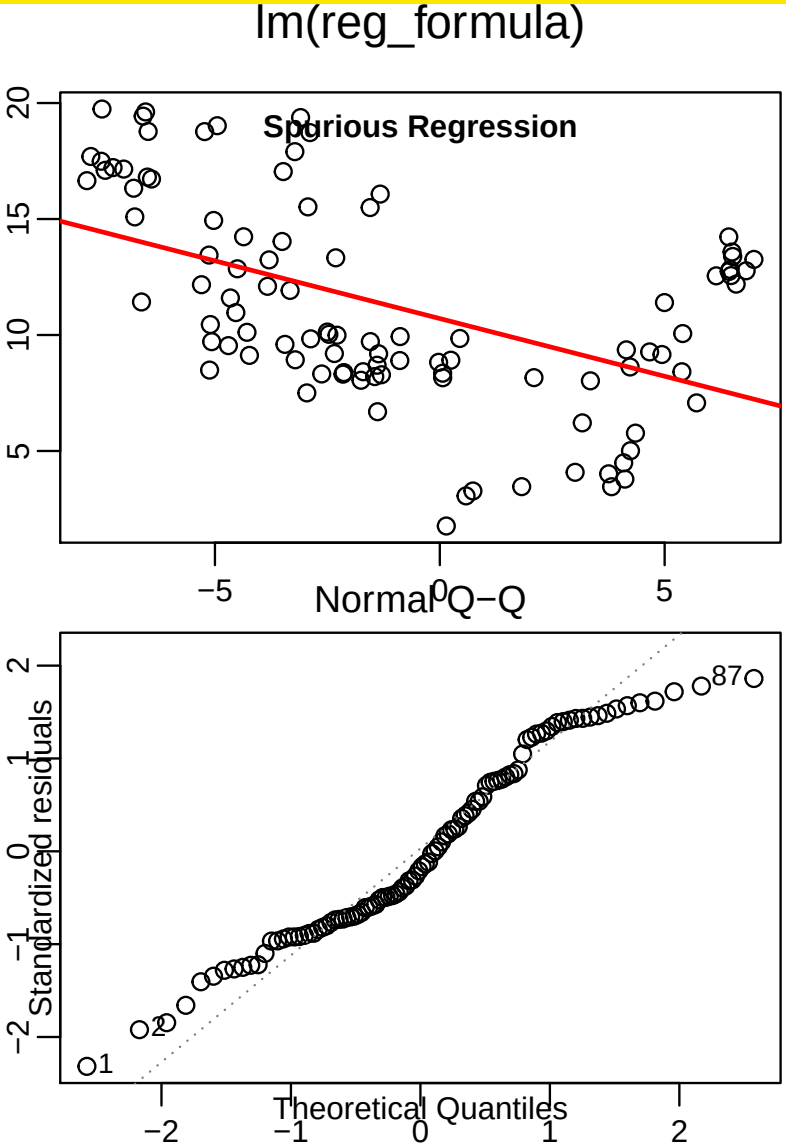
But the failure of the Durbin-Watson test doesn't reject the existence of a linear relationship between the response and predictor variables, it just puts it in doubt.

Links:
https://onlinecourses.science.psu.edu/stat510/node/72
http://stats.stackexchange.com/questions/6469/simple-linear-model-with-autocorrelated-errors-in-r

Regression of non-stationary time series creates *spurious* regressions.

The *t*-statistics, *p*-values, and *R*-squared all indicate a statistically significant regression.

But the Durbin-Watson test shows residuals are



The *Leverage* for Univariate Regression

We can add an extra unit column to the *predictor matrix* $\mathbb{X}$ so that the univariate regression can be written in *homogeneous form* as:

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

With two *regression coefficients*: $\beta = (\alpha, \beta_1)$, and a *predictor matrix* $\mathbb{X}$ with two columns, with the first column equal to a unit vector.

After the second column of the *predictor matrix* $\mathbb{X}$ is centered (de-meaned), its *covariance matrix* is given by:

$$\mathbb{X}^T\mathbb{X} = \begin{pmatrix} n & 0 \\ 0 & \sum_{i=1}^{n}(x_i - \bar{x})^2 \end{pmatrix}$$

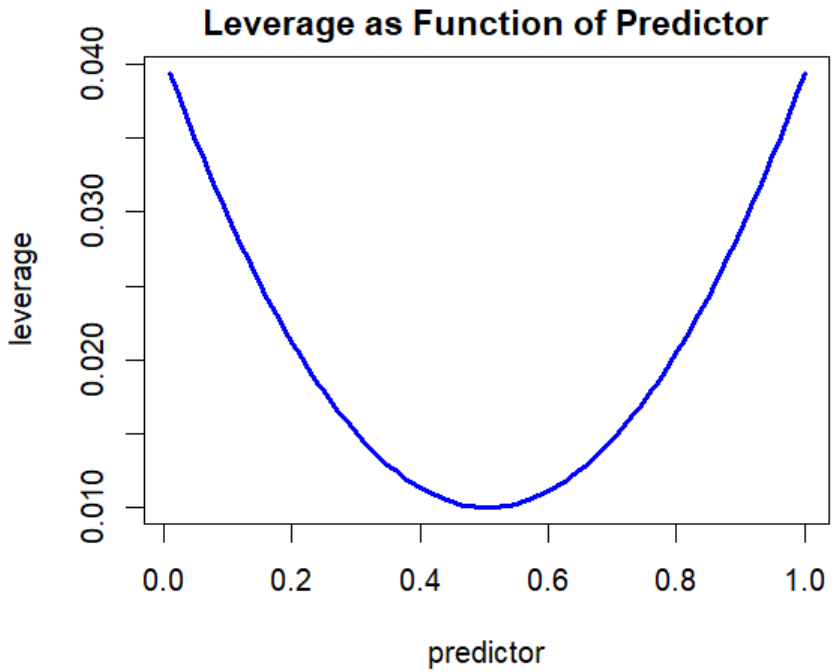
And the *influence matrix* $\mathbb{H}$ is given by:

$$\mathbb{H}_{ij} = [\mathbb{X}(\mathbb{X}^T\mathbb{X})^{-1}\mathbb{X}^T]_{ij} = \frac{1}{n} + \frac{(x_i - \bar{x})(x_j - \bar{x})}{\sum_{i=1}^{n}(x_i - \bar{x})^2}$$

The first term above is due to the influence of the regression intercept α, and the second term is due to the influence of the regression slope β_1.

The diagonal elements of the *influence matrix* $\mathbb{H}_{ii}$ form the *leverage vector*.

```
> # Define linear regression data
> # Initialize the random number generator
> set.seed(1121, "Mersenne-Twister", sample.kind="Rejection")
> nrows <- 100
> predm <- runif(nrows)
> noisey <- rnorm(nrows)
```




```
> # Add unit column to the predictor matrix
> predm <- cbind(rep(1, nrows), predm)
> # Calculate the generalized inverse of the predictor matrix
> predinv <- MASS::ginv(predm)
> # Calculate the influence matrix
> infmat <- predm %*% predinv
> # Plot the leverage vector
> ordern <- order(predm[, 2])
> plot(x=predm[ordern, 2], y=diag(infmat)[ordern],
+      type="l", lwd=3, col="blue",
+      xlab="predictor", ylab="leverage",
+      main="Leverage as Function of Predictor")
```

Covariance Matrix of Fitted Values in Univariate Regression

The *fitted values* y_{fit} can be considered to be *random variables* $\hat{y}_{fit}$:

$$\hat{y}_{fit} = \mathbb{H}\hat{y} = \mathbb{H}(y_{fit} + \hat{\varepsilon}) = y_{fit} + \mathbb{H}\hat{\varepsilon}$$

The *covariance matrix* of the *fitted values* $\hat{y}_{fit}$ is:

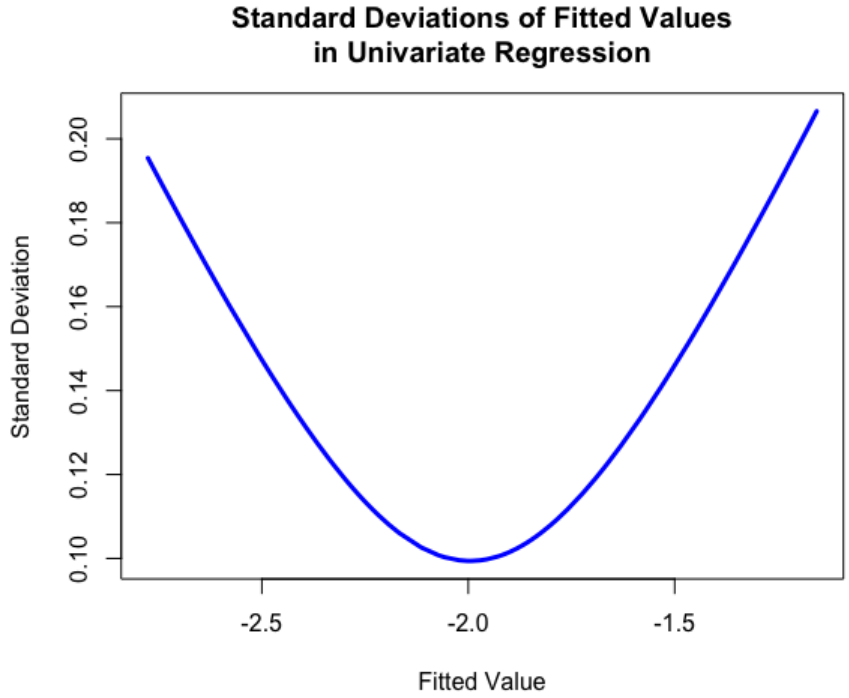
$$\sigma^2_{fit} = \frac{\mathbb{E}[\mathbb{H}\hat{\varepsilon}(\mathbb{H}\hat{\varepsilon})^T]}{d_{free}} = \frac{\mathbb{E}[\mathbb{H}\,\hat{\varepsilon}\hat{\varepsilon}^T\mathbb{H}^T]}{d_{free}} = \frac{\mathbb{H}\,\mathbb{E}[\hat{\varepsilon}\hat{\varepsilon}^T]\,\mathbb{H}^T}{d_{free}} = \sigma^2_{\varepsilon}\,\mathbb{H}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

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^2_{fit} 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
> infmat <- predm %*% predinv
> # The influence matrix is idempotent
> all.equal(infmat, infmat %*% infmat)
```




```
> # Calculate the covariance and standard deviations of fitted value
> betac <- predinv %*% respv
> fitv <- drop(predm %*% betac)
> resids <- drop(respv - fitv)
> degf <- (NROW(predm) - NCOL(predm))
> residsd <- sqrt(sum(resids^2)/degf)
> fitcovar <- residsd*infmat
> fitsd <- sqrt(diag(fitcovar))
> # Plot the standard deviations
> fitdata <- cbind(fitted=fitv, stdev=fitsd)
> fitdata <- fitdata[order(fitv), ]
> plot(fitdata, type="l", lwd=3, col="blue",
+      xlab="Fitted Value", ylab="Standard Deviation",
+      main="Standard Deviations of Fitted Values\nin Univariate Reg
```

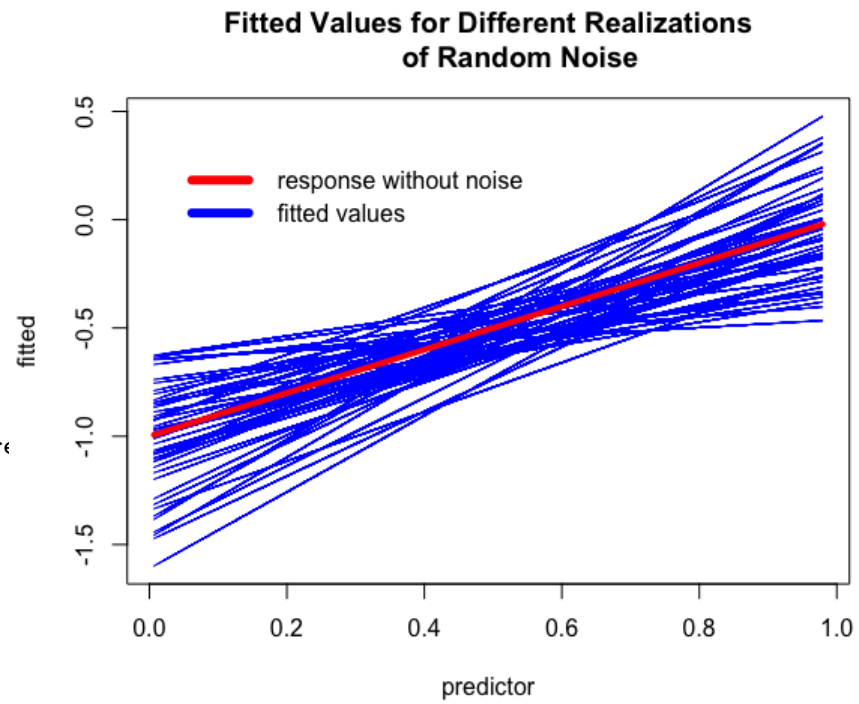
Fitted Values for Different Realizations of Random Noise

The fitted values are more volatile for *predictor* values that are further away from their mean, because those points have higher *leverage*.

The higher *leverage* of points further away from the mean of the *predictor* is due to their greater sensitivity to changes in the slope of the regression.

The fitted values for different realizations of random noise can be calculated using the influence matrix.

```
> # Calculate the response without random noise for univariate regre
> # equal to weighted sum over columns of predictor.
> respn <- predm %*% c(-1, 1)
> # Perform loop over different realizations of random noise
> fitm <- lapply(1:50, function(it) {
+   # Add random noise to response
+   respv <- respn + rnorm(nrows, sd=1.0)
+   # Calculate the fitted values using influence matrix
+   infmat %*% respv
+ })  # end lapply
> fitm <- rutils::do_call(cbind, fitm)
```




```
> # Plot fitted values
> matplot(x=predm[, 2], y=fitm,
+ type="l", lty="solid", lwd=1, col="blue",
+ xlab="predictor", ylab="fitted",
+ main="Fitted Values for Different Realizations
+ of Random Noise")
> lines(x=predm[, 2], y=respn, col="red", lwd=4)
> legend(x="topleft", # Add legend
+        legend=c("response without noise", "fitted values"),
+        title=NULL, inset=0.05, cex=1.0, lwd=6, y.intersp=0.4,
+        bty="n", lty=1, col=c("red", "blue"))
```

Forecasts From *Univariate Regression* Models

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

$$y_f = \mathbb{X}_{new}\,\beta$$

The variance σ_f^2 of the *forecast value* is equal to the *predictor* vector multiplied by the *covariance matrix* of the *regression coefficients* σ_β^2:

$$\sigma_f^2 = \frac{\mathbb{E}[\mathbb{X}_{new}\mathbb{X}_{inv}\hat{\varepsilon}\,(\mathbb{X}_{new}\mathbb{X}_{inv}\hat{\varepsilon})^T]}{d_{free}} =$$

$$\frac{\mathbb{E}[\mathbb{X}_{new}\mathbb{X}_{inv}\hat{\varepsilon}\hat{\varepsilon}^T\mathbb{X}_{inv}^T\mathbb{X}_{new}^T]}{d_{free}} = \sigma_\varepsilon^2\mathbb{X}_{new}\mathbb{X}_{inv}\mathbb{X}_{inv}^T\mathbb{X}_{new}^T =$$

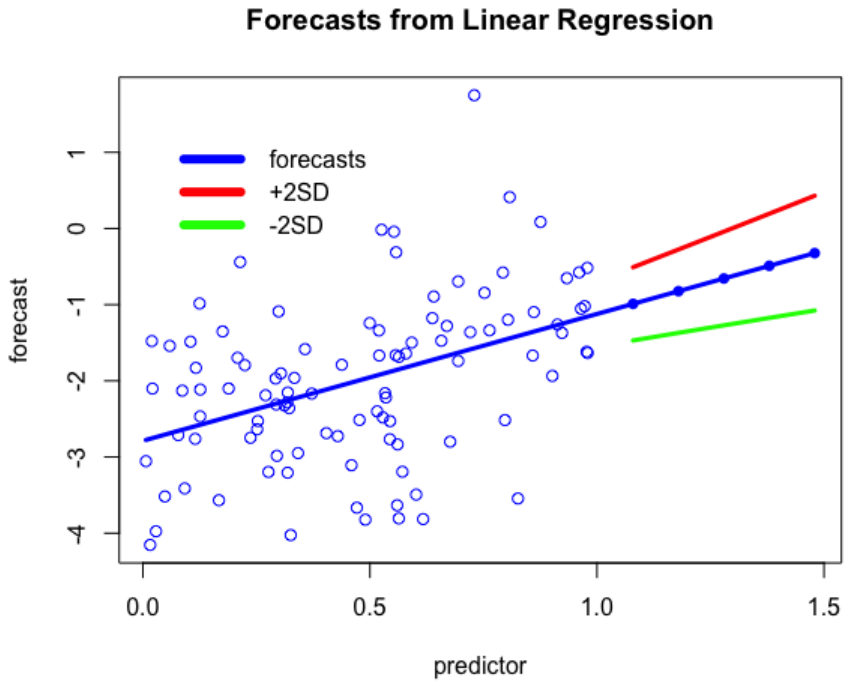
$$\sigma_\varepsilon^2\,\mathbb{X}_{new}(\mathbb{X}^T\mathbb{X})^{-1}\mathbb{X}_{new}^T = \mathbb{X}_{new}\,\sigma_\beta^2\,\mathbb{X}_{new}^T$$

```
> # Define new predictor
> newdata <- (max(predm[, 2]) + 10*(1:5)/nrows)
> predn <- cbind(rep(1, NROW(newdata)), newdata)
> # Calculate the forecast values
> fcast <- drop(predn %*% betac)
> # Calculate the inverse of the predictor matrix squared
> pred2 <- MASS::ginv(crossprod(predm))
> # Calculate the standard errors
> predsd <- residsd*sqrt(predn %*% pred2 %*% t(predn))
> # Combine the forecast values and standard errors
> fcast <- cbind(forecast=fcast, stdev=diag(predsd))
```

Confidence Intervals of Regression Forecasts

The variables σ_ε^2 and σ_y^2 follow the *chi-squared* distribution with $d_{free} = (n - k - 1)$ degrees of freedom, so the *forecast value* y_f follows the *t-distribution*.

```
> # Prepare plot data
> xdata <- c(predm[, 2], newdata)
> ydata <- c(fitv, fcast[, 1])
> # Calculate the t-quantile
> tquant <- qt(pnorm(2), df=degf)
> fcastl <- fcast[, 1] - tquant*fcast[, 2]
> fcasth <- fcast[, 1] + tquant*fcast[, 2]
> # Plot the regression forecasts
> xlim <- range(xdata)
> ylim <- range(c(respv, ydata, fcastl, fcasth))
> plot(x=xdata, y=ydata, xlim=xlim, ylim=ylim,
+      type="l", lwd=3, col="blue",
+      xlab="predictor", ylab="forecast",
+      main="Forecasts from Linear Regression")
> points(x=predm[, 2], y=respv, col="blue")
> points(x=newdata, y=fcast[, 1], pch=16, col="blue")
> lines(x=newdata, y=fcasth, lwd=3, col="red")
> lines(x=newdata, y=fcastl, lwd=3, col="green")
> legend(x="topleft", # Add legend
+        legend=c("forecasts", "+2SD", "-2SD"),
+        title=NULL, inset=0.05, cex=1.0, lwd=6, y.intersp=0.4,
+        bty="n", lty=1, col=c("blue", "red", "green"))
```

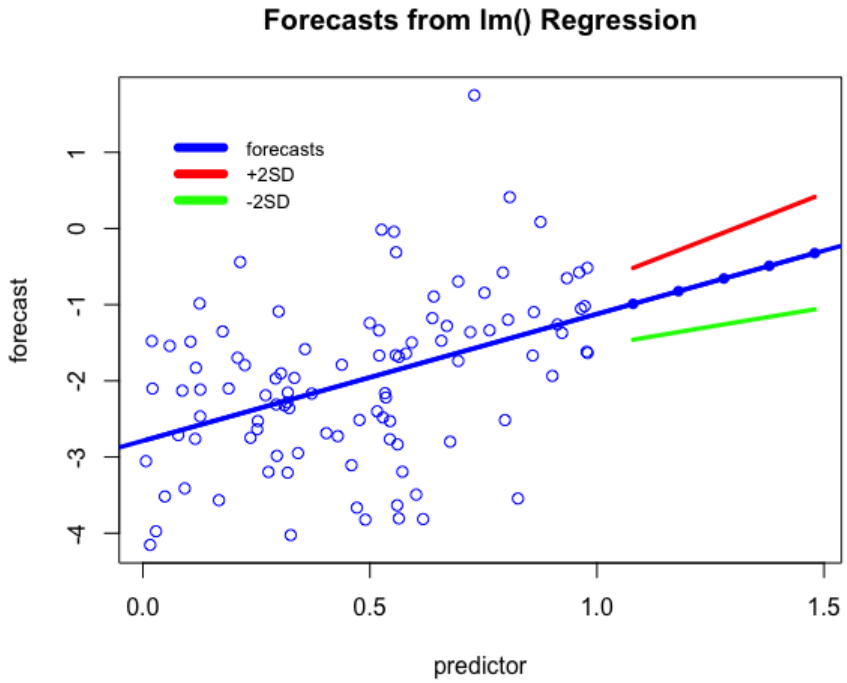


Forecasts of *Linear Regression* Using `predict.lm()`

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

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

```
> # Perform univariate regression
> dframe <- data.frame(resp=respv, pred=predm[, 2])
> regmod <- lm(resp ~ pred, data=dframe)
> # Calculate the forecasts from regression
> newdf <- data.frame(pred=predn[, 2]) # Same column name
> fcastlm <- predict.lm(object=regmod,
+   newdata=newdf, confl=1-2*(1-pnorm(2)),
+   interval="confidence")
> rownames(fcastlm) <- NULL
> all.equal(fcastlm[, "fit"], fcast[, 1])
> all.equal(fcastlm[, "lwr"], fcastl)
> all.equal(fcastlm[, "upr"], fcasth)
> plot(x=xdata, y=ydata, xlim=xlim, ylim=ylim,
+      type="l", lwd=3, col="blue",
+      xlab="predictor", ylab="forecast",
+      main="Forecasts from lm() Regression")
> points(x=predm[, 2], y=respv, col="blue")
```




```
> abline(regmod, col="blue", lwd=3)
> points(x=newdata, y=fcastlm[, "fit"], pch=16, col="blue")
> lines(x=newdata, y=fcastlm[, "lwr"], lwd=3, col="green")
> lines(x=newdata, y=fcastlm[, "upr"], lwd=3, col="red")
> legend(x="topleft", # Add legend
+        legend=c("forecasts", "+2SD", "-2SD"),
+        title=NULL, inset=0.05, cex=0.8, lwd=6, y.intersp=0.4,
+        bty="n", lty=1, col=c("blue", "red", "green"))
```

Spurious Time Series Regression

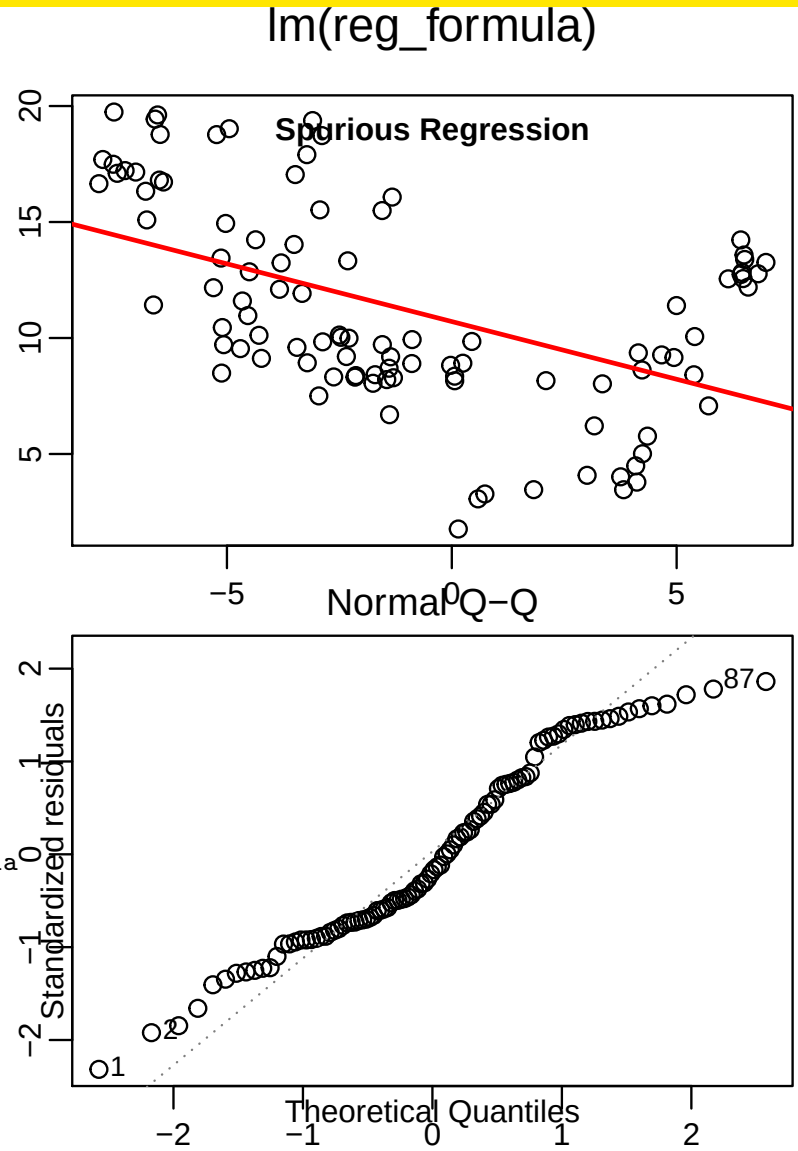
Regression of non-stationary time series creates *spurious* regressions.

The *t*-statistics, *p*-values, and *R*-squared all indicate a statistically significant regression.

But the Durbin-Watson test shows residuals are autocorrelated, which invalidates the other tests.

The Q-Q plot also shows that residuals are *not* normally distributed.

```
> predm <- cumsum(rnorm(100))  # Unit root time series
> respv <- cumsum(rnorm(100))
> formulav <- respv ~ predm
> regmod <- lm(formulav)  # Perform regression
> # Summary indicates statistically significant regression
> regsum <- summary(regmod)
> regsum$coeff
> regsum$r.squared
> # Durbin-Watson test shows residuals are autocorrelated
> dwtest <- lmtest::dwtest(regmod)
> c(dwtest$statistic[[1]], dwtest$p.value)
> plot(formulav, xlab="", ylab="")  # Plot scatterplot using formula
> title(main="Spurious Regression", line=-1)
> # Add regression line
> abline(regmod, lwd=2, col="red")
> plot(regmod, which=2, ask=FALSE)  # Plot just Q-Q
```



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
> # Initialize the random number generator
> set.seed(1121, "Mersenne-Twister", sample.kind="Rejection")
> predm <- matrix(runif(nrows*ncols), ncol=ncols)
> # Add column names
> colnames(predm) <- paste0("pred", 1:ncols)
> # Define the predictor weights
> weightv <- runif(3:(ncols+2), min=(-1), max=1)
> # Response equals weighted predictor plus random noise
> noisev <- rnorm(nrows, sd=2)
> respv <- (1 + predm %*% weightv + noisev)
```

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:

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

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 centered (de-meaned) variables.

The matrix $\hat{\mathbb{X}}^{inv}$ is the generalized inverse of the centered (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(respv ~ predm)
> # Solve multivariate regression using matrix algebra
> # Calculate the centered (de-meaned) predictor matrix and response
> # predc <- t(t(predm) - colMeans(predm))
> predc <- apply(predm, 2, function(x) (x-mean(x)))
> respc <- respv - mean(respv)
> # Calculate the regression coefficients
> betac <- drop(MASS::ginv(predc) %*% respc)
> # Calculate the regression alpha
> alphac <- mean(respv) - sum(colSums(predm)*betac)/nrows
> # Compare with coefficients from lm()
> all.equal(coef(regmod), c(alphac, betac), check.attributes=FALSE)
[1] TRUE
> # Compare with actual coefficients
> all.equal(c(1, weightv), c(alphac, betac), check.attributes=FALSE)
[1] "Mean relative difference: 0.963"
```

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: $\beta = (\alpha, \beta_1, \ldots, \beta_k)$, 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
> predm <- cbind(rep(1, nrows), predm)
> ncols <- NCOL(predm)
> # Add column name
> colnames(predm)[1] <- "intercept"
> # Calculate the generalized inverse of the predictor matrix
> predinv <- MASS::ginv(predm)
> # Calculate the regression coefficients
> betac <- predinv %*% respv
> # Perform multivariate regression without intercept term
> regmod <- lm(respv ~ predm - 1)
> all.equal(drop(betac), coef(regmod), check.attributes=FALSE)
[1] TRUE
```

The *Residuals* of Multivariate Regression

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

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

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* $\mathbb{X}$ (the *predictors*):

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

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

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

```
> # Calculate the fitted values from regression coefficients
> fitv <- drop(predm %*% betac)
> all.equal(fitv, regmod$fitted.values, check.attributes=FALSE)
[1] TRUE
> # Calculate the residuals
> resids <- drop(respv - fitv)
> all.equal(resids, regmod$residuals, check.attributes=FALSE)
[1] TRUE
> # Residuals are orthogonal to predictor columns (predms)
> sapply(resids %*% predm, all.equal, target=0)
[1] TRUE TRUE TRUE TRUE TRUE TRUE
> # Residuals are orthogonal to the fitted values
> all.equal(sum(resids*fitv), target=0)
[1] TRUE
> # Sum of residuals is equal to zero
> all.equal(sum(resids), 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
> infmat <- predm %*% predinv
> # The influence matrix is idempotent
> all.equal(infmat, infmat %*% infmat)
[1] TRUE
> # Calculate the fitted values using influence matrix
> fitv <- drop(infmat %*% respv)
> all.equal(fitv, regmod$fitted.values, check.attributes=FALSE)
[1] TRUE
> # Calculate the fitted values from regression coefficients
> fitv <- drop(predm %*% betac)
> all.equal(fitv, regmod$fitted.values, check.attributes=FALSE)
[1] TRUE
```

Multivariate Regression With Centered 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 centered (de-meaned) response and predictor matrix:

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

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

The regression model with a centered (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.

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

```
> # Calculate the centered (de-meaned) fitted values
> predc <- t(t(predm) - colMeans(predm))
> fittedc <- drop(predc %*% betac)
> all.equal(fittedc, regmod$fitted.values - mean(respv),
+   check.attributes=FALSE)
[1] TRUE
> # Calculate the residuals
> respc <- respv - mean(respv)
> resids <- drop(respc - fittedc)
> all.equal(resids, regmod$residuals, check.attributes=FALSE)
[1] TRUE
> # Calculate the influence matrix
> infmatc <- predc %*% MASS::ginv(predc)
> # Compare the fitted values
> all.equal(fittedc, drop(infmatc %*% respc), check.attributes=FALSE
[1] TRUE
```

Multivariate Regression for Orthogonal Predictors

The generalized inverse can be written as:

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

Where $\mathbb{C} = \mathbb{X}^T\mathbb{X}$ is the matrix of inner products of the predictors $\mathbb{X}$.

If the predictors are orthogonal ($x_i \cdot x_j = 0$ for $i \neq j$, and $x_i \cdot x_i = \sigma_i^2$) then the squared predictor matrix $\mathbb{C}$ is diagonal:

$$\mathbb{C} = \begin{pmatrix} \sigma_1^2 & 0 & \cdots & 0 \\ 0 & \sigma_2^2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \sigma_n^2 \end{pmatrix}$$

And the inverse of the squared predictor matrix $\mathbb{C}^{-1}$ is also diagonal, so the *regression coefficients* can then be written simply as:

$$\beta_i = \frac{x_i \cdot y}{\sigma_i^2}$$

Where $x_i \cdot y$ are the inner products of the predictors x_i times the *response vector* y.

Conversely, if the predictors are *collinear* then their squared predictor matrix is *singular* and the regression is also singular. Predictors are *collinear* if there's a linear combination that is constant.

```
> # Perform PCA of the predictors
> pcad <- prcomp(predm, center=FALSE, scale=FALSE)
> # Calculate the PCA predictors
> predpca <- predm %*% pcad$rotation
> # Principal components are orthogonal to each other
> round(t(predpca) %*% predpca, 2)
> # Calculate the PCA regression coefficients using lm()
> regmod <- lm(respv ~ predpca - 1)
> summary(regmod)
> regmod$coefficients
> # Calculate the PCA regression coefficients directly
> colSums(predpca*drop(respv))/colSums(predpca^2)
> # Create almost collinear predictors
> predcol <- predm
> predcol[, 1] <- (predcol[, 1]/1e3 + predcol[, 2])
> # Calculate the PCA predictors
> pcad <- prcomp(predcol, center=FALSE, scale=FALSE)
> predpca <- predcol %*% pcad$rotation
> round(t(predpca) %*% predpca, 6)
> # Calculate the PCA regression coefficients
> drop(MASS::ginv(predpca) %*% respv)
> # Calculate the PCA regression coefficients directly
> colSums(predpca*drop(respv))/colSums(predpca^2)
```

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*:

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

Where $d_{free} = (n - k)$ 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* $\hat{\varepsilon}$:

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

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

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

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

```
> # Regression model summary
> regsum <- summary(regmod)
> # Degrees of freedom of residuals
> nrows <- NROW(predm)
> ncols <- NCOL(predm)
> degf <- (nrows - ncols)
> all.equal(degf, regsum$df[2])
[1] TRUE
> # Variance of residuals
> residsd <- sum(resids^2)/degf
```

Covariance Matrix of the Regression Coefficients

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

$$\sigma_{\beta}^2 = \frac{\mathbb{E}[(\hat{\beta} - \beta)(\hat{\beta} - \beta)^T]}{d_{free}} =$$

$$\frac{\mathbb{E}[\mathbb{X}_{inv}\hat{\varepsilon}(\mathbb{X}_{inv}\hat{\varepsilon})^T]}{d_{free}} = \frac{\mathbb{E}[\mathbb{X}_{inv}\hat{\varepsilon}\hat{\varepsilon}^T\mathbb{X}_{inv}^T]}{d_{free}} =$$

$$\frac{(\mathbb{X}^T\mathbb{X})^{-1}\mathbb{X}^T\mathbb{E}[\hat{\varepsilon}\hat{\varepsilon}^T]\,\mathbb{X}(\mathbb{X}^T\mathbb{X})^{-1}}{d_{free}} =$$

$$(\mathbb{X}^T\mathbb{X})^{-1}\mathbb{X}^T\sigma_{\varepsilon}^2\mathbb{1}\,\mathbb{X}(\mathbb{X}^T\mathbb{X})^{-1} = \sigma_{\varepsilon}^2(\mathbb{X}^T\mathbb{X})^{-1}$$

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

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

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

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

```
> # Inverse of predictor matrix squared
> pred2 <- MASS::ginv(crossprod(predm))
> # pred2 <- t(predm) %*% predm
> # Variance of residuals
> residsd <- sum(resids^2)/degf
> # Calculate the covariance matrix of betas
> betacovar <- residsd*pred2
> # round(betacovar, 3)
> betasd <- sqrt(diag(betacovar))
> all.equal(betasd, regsum$coeff[, 2], check.attributes=FALSE)
[1] TRUE
> # Calculate the t-values of betas
> betatvals <- drop(betac)/betasd
> all.equal(betatvals, regsum$coeff[, 3], check.attributes=FALSE)
[1] TRUE
> # Calculate the two-sided p-values of betas
> betapvals <- 2*pt(-abs(betatvals), df=degf)
> all.equal(betapvals, regsum$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(predm)), predinv %*% t(predinv))
[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*:
$\hat{y}_{fit} = \mathbb{X}\hat{\beta} = \mathbb{X}(\beta + \mathbb{X}_{inv}\hat{\varepsilon}) = y_{fit} + \mathbb{X}\mathbb{X}_{inv}\hat{\varepsilon}$.

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

$$\sigma^2_{fit} = \frac{\mathbb{E}[\mathbb{X}\mathbb{X}_{inv}\hat{\varepsilon}\,(\mathbb{X}\mathbb{X}_{inv}\hat{\varepsilon})^T]}{d_{free}} = \frac{\mathbb{E}[\mathbb{H}\,\hat{\varepsilon}\hat{\varepsilon}^T\mathbb{H}^T]}{d_{free}} =$$

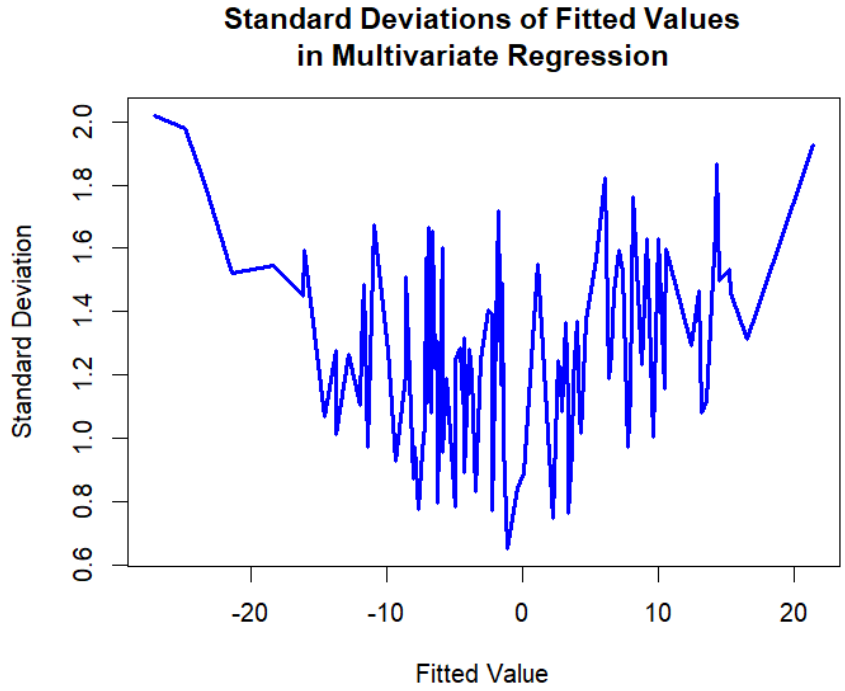
$$\frac{\mathbb{H}\,\mathbb{E}[\hat{\varepsilon}\hat{\varepsilon}^T]\,\mathbb{H}^T}{d_{free}} = \sigma^2_{\varepsilon}\,\mathbb{H} = \sigma^2_{\varepsilon}\,\mathbb{X}(\mathbb{X}^T\mathbb{X})^{-1}\mathbb{X}^T$$

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^2_{fit} 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
> infmat <- predm %*% predinv
> # The influence matrix is idempotent
> all.equal(infmat, infmat %*% infmat)
```




```
> # Calculate the covariance and standard deviations of fitted value
> fitcovar <- residsd*infmat
> fitsd <- sqrt(diag(fitcovar))
> # Sort the standard deviations
> fitsd <- cbind(fitted=fitv, stdev=fitsd)
> fitsd <- fitsd[order(fitv), ]
> # 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 R
```

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
> retp <- rutils::etfenv$returns[, c("XLF", "XLE")]
> retp <- na.omit(retp)
> nrows <- NROW(retp)
> head(retp)
> # Define regression formula
> formulav <- paste(colnames(retp)[1],
+   paste(colnames(retp)[-1], collapse="+"),
+   sep=" ~ ")
> # Standard regression
> regmod <- lm(formulav, data=retp)
> regsum <- summary(regmod)
> # Bootstrap of regression
> # Initialize the random number generator
> set.seed(1121, "Mersenne-Twister", sample.kind="Rejection")
> bootd <- sapply(1:100, function(x) {
+   samplev <- sample.int(nrows, replace=TRUE)
+   regmod <- lm(formulav, data=retp[samplev, ])
+   regmod$coefficients
+ })  # end sapply
> # Means and standard errors from regression
> regsum$coefficients
> # Means and standard errors from bootstrap
> dim(bootd)
> t(apply(bootd, MARGIN=1,
+ function(x) c(mean=mean(x), stderror=sd(x))))
```

Forecasts From Multivariate Regression Models

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

$$y_f = \mathbb{X}_{new}\, \beta$$

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

$$\hat{y}_f = \mathbb{X}_{new}\hat{\beta} = \mathbb{X}_{new}(\beta + \mathbb{X}_{inv}\hat{\varepsilon}) = y_f + \mathbb{X}_{new}\mathbb{X}_{inv}\hat{\varepsilon}$$

The variance σ_f^2 of the *forecast value* is:

$$\sigma_f^2 = \frac{\mathbb{E}[\mathbb{X}_{new}\mathbb{X}_{inv}\hat{\varepsilon}\,(\mathbb{X}_{new}\mathbb{X}_{inv}\hat{\varepsilon})^T]}{d_{free}} = \frac{\mathbb{E}[\mathbb{X}_{new}\mathbb{X}_{inv}\hat{\varepsilon}\hat{\varepsilon}^T\mathbb{X}_{inv}^T\mathbb{X}_{new}^T]}{d_{free}} =$$

$$\sigma_\varepsilon^2\mathbb{X}_{new}\mathbb{X}_{inv}\mathbb{X}_{inv}^T\mathbb{X}_{new}^T =$$

$$\sigma_\varepsilon^2\,\mathbb{X}_{new}(\mathbb{X}^T\mathbb{X})^{-1}\mathbb{X}_{new}^T = \mathbb{X}_{new}\,\sigma_\beta^2\,\mathbb{X}_{new}^T$$

The variance σ_f^2 of the *forecast 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, "Mersenne-Twister", sample.kind="Rejection")
> newdata <- data.frame(matrix(c(1, rnorm(5)), nr=1))
> colnamev <- colnames(predm)
> colnames(newdata) <- colnamev
> newdata <- as.matrix(newdata)
> fcast <- drop(newdata %*% betac)
> predsd <- drop(sqrt(newdata %*% betacovar %*% t(newdata)))
```

Forecasts From Multivariate Regression Using lm()

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

predict.lm() is the forecasting 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("respv ~ ",
+   paste(colnames(predm), collapse=" + "), " - 1")
> # Specify multivariate regression using formula
> regmod <- lm(formulav, data=data.frame(cbind(respv, predm)))
> regsum <- summary(regmod)
> # Predict from lm object
> fcastlm <- predict.lm(object=model, newdata=newdata,
+    interval="confidence", confl=1-2*(1-pnorm(2)))
> # Calculate the t-quantile
> tquant <- qt(pnorm(2), df=degf)
> fcasth <- (fcast + tquant*predsd)
> fcastl <- (fcast - tquant*predsd)
> # Compare with matrix calculations
> all.equal(fcastlm[1, "fit"], fcast)
> all.equal(fcastlm[1, "lwr"], fcastl)
> all.equal(fcastlm[1, "upr"], fcasth)
```

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 $(y_{fit} - \bar{y})$:

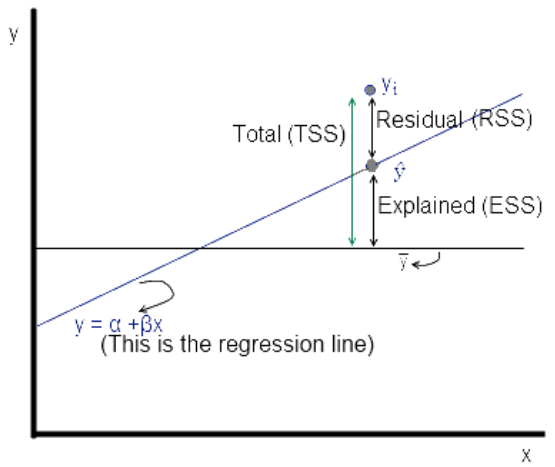
$$(y - y_{fit})^T (y_{fit} - \bar{y}) = 0$$

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



$\hat{y}$ is the predicted value of y given x, using the equation $\hat{y} = \alpha + \beta x$.

y_i is the actual observed value of y

$\bar{y}$ is the mean of y.

The distances that RSS, ESS and TSS represent are shown in the diagram to the left - but remember that the actual calculations are squares of these distances.

$$TSS = \Sigma (y_i - \bar{y})^2$$

$$RSS = \Sigma (y_i - \hat{y})^2$$

$$ESS = \Sigma (\hat{y} - \bar{y})^2$$

```
> # TSS = ESS + RSS
> tss <- sum((respv-mean(respv))^2)
> ess <- sum((fitv-mean(fitv))^2)
> rss <- sum(resids^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*:

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

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

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

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

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(predm)
> ncols <- NCOL(predm)
> # Degrees of freedom of residuals
> degf <- (nrows - ncols)
> # Adjusted R-squared
> rsqadj <- (1-sum(resids^2)/degf/var(respv))
> # Compare adjusted R-squared from lm()
> all.equal(drop(rsqadj), regsum$adj.r.squared)
[1] TRUE
```

Fisher's *F-distribution*

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

Then the random variable:

$$F = \frac{\chi^2_m / m}{\chi^2_n / n}$$

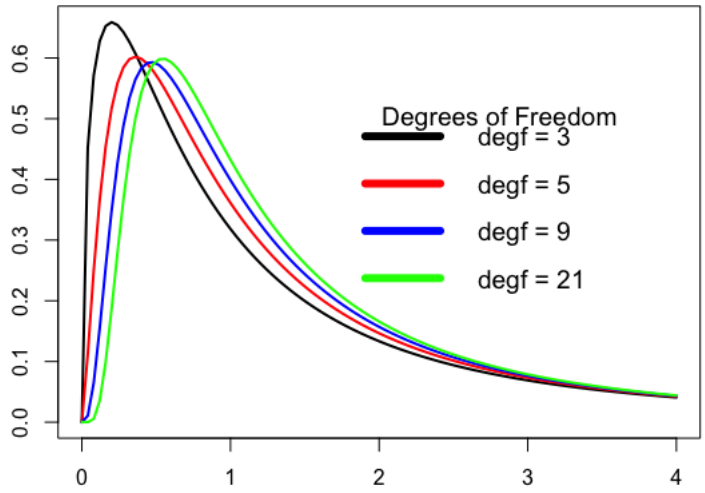
Follows the *F-distribution* with m and n degrees of freedom, with the probability density function:

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

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

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

```
> # Plot four curves in loop
> degf <- c(3, 5, 9, 21)  # Degrees of freedom
> colorv <- c("black", "red", "blue", "green")
> for (indeks in 1:NROW(degf)) {
+   curve(expr=df(x, df1=degf[indeks], df2=3),
+     xlim=c(0, 4), xlab="", ylab="", lwd=2,
+     col=colorv[indeks], add=as.logical(indeks-1))
+ }  # end for
```




```
> # Add title
> title(main="F-Distributions", line=0.5)
> # Add legend
> labelv <- paste("degf", degf, sep=" = ")
> legend("topright", title="Degrees of Freedom", inset=0.0, bty="n",
+        y.intersp=0.4, labelv, cex=1.2, lwd=6, lty=1, col=colorv)
```

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 *null hypothesis* of the *F-test* test is 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 fratios
> 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 $p_1 > p_2$.

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 has only 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* $ESS = (y_{fit} - \bar{y})^T (y_{fit} - \bar{y})$ 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).

The *null hypothesis* of the *F-test* test is that the *F-statistic* F is not significantly greater than 1 (the variance of *ESS* is not significantly greater than of *RSS*).

A large value of the *F-statistic* F indicates that the variance of *ESS* is significantly greater than that of *RSS*, and that the regression is statistically significant.

```
> # F-statistic from lm()
> regsum$fstatistic
value numdf dendf
 3.37  5.00 94.00
> # Degrees of freedom of residuals
> degf <- (nrows - ncols)
> # F-statistic from ESS and RSS
> fstat <- (ess/(ncols-1))/(rss/degf)
> all.equal(fstat, regsum$fstatistic[1], check.attributes=FALSE)
[1] TRUE
> # p-value of F-statistic
> 1-pf(q=fstat, df1=(ncols-1), df2=(nrows-ncols))
[1] 0.00757
```

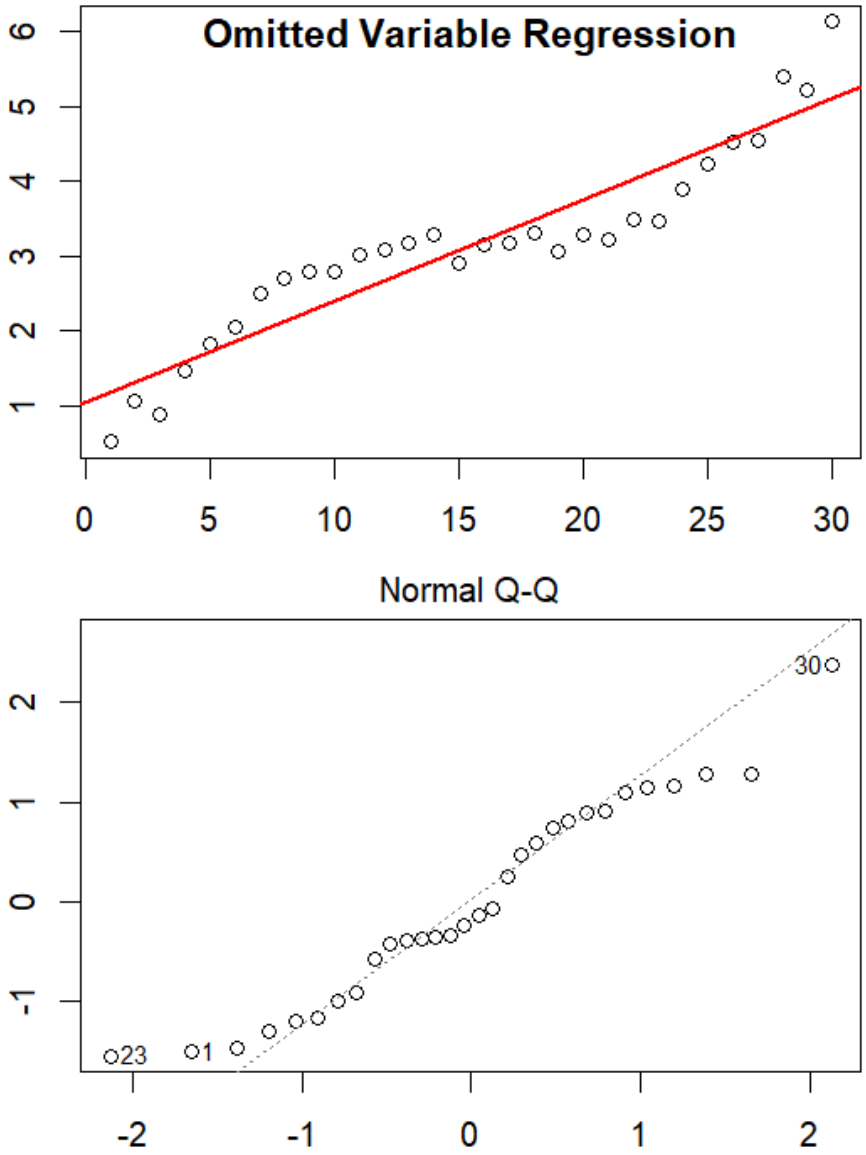
Omitted Variable Bias

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
> predm <- 1:30
> omitv <- sin(0.2*1:30)
> # Response depends on both predictors
> respv <- 0.2*predm + omitv + 0.2*rnorm(30)
> # Mis-specified regression only one predictor
> modovb <- lm(respv ~ predm)
> regsum <- summary(modovb)
> regsum$coeff
> regsum$r.squared
> # Durbin-Watson test shows residuals are autocorrelated
> lmtest::dwtest(modovb)
> # 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(respv ~ predm)
> abline(modovb, lwd=2, col="red")
> title(main="Omitted Variable Regression", line=-1)
> plot(modovb, which=2, ask=FALSE)  # Plot just Q-Q
```



Regularized Inverse of Rectangular Matrices

The *SVD* of a rectangular matrix $\mathbb{A}$ is defined as the factorization:

$$\mathbb{A} = \mathbb{U}\mathbf{\Sigma}\mathbb{V}^T$$

Where $\mathbb{U}$ and $\mathbb{V}$ are the *singular matrices*, and $\mathbf{\Sigma}$ is a diagonal matrix of *singular values*.

The *generalized inverse* matrix $\mathbb{A}^{-1}$ satisfies the inverse equation: $\mathbb{A}\mathbb{A}^{-1}\mathbb{A} = \mathbb{A}$, and it can be expressed as a product of the *SVD* matrices as follows:

$$\mathbb{A}^{-1} = \mathbb{V}\,\mathbf{\Sigma}^{-1}\,\mathbb{U}^T$$

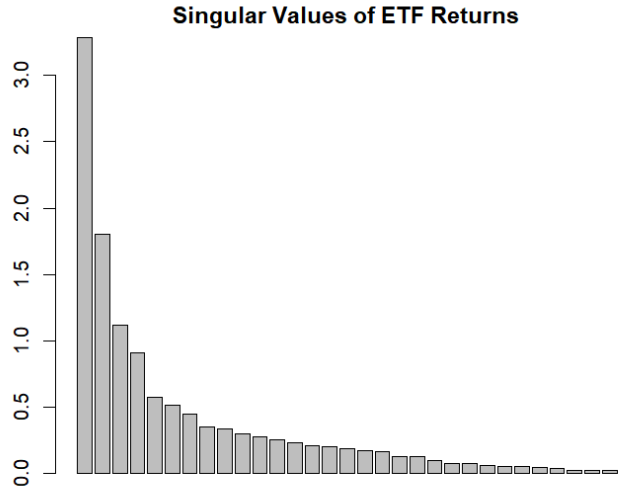
If any of the *singular values* are zero then the *generalized inverse* does not exist.

The *regularized inverse* is obtained by removing very small *singular values*:

$$\mathbb{A}^{-1} = \mathbb{V}_n\,\mathbf{\Sigma}_n^{-1}\,\mathbb{U}_n^T$$

Where $\mathbb{U}_n$, $\mathbb{V}_n$ and $\mathbf{\Sigma}_n$ are the *SVD* matrices without very small *singular values*.

The regularized inverse satisfies the inverse equation only approximately (it has *bias*), but it's often used in machine learning because it has lower *variance* than the exact inverse.




```
> # Calculate the ETF returns
> retp <- na.omit(rutils::etfenv$returns)
> # Perform singular value decomposition
> svdec <- svd(retp)
> barplot(svdec$d, main="Singular Values of ETF Returns")
```

```
> # Calculate the generalized inverse from SVD
> invmat <- svdec$v %*% (t(svdec$u) / svdec$d)
> # Verify inverse property of inverse
> all.equal(zoo::coredata(retp), retp %*% invmat %*% retp)
> # Calculate the regularized inverse from SVD
> dimax <- 1:3
> invreg <- svdec$v[, dimax] %*%
+   (t(svdec$u[, dimax]) / svdec$d[dimax])
> # Calculate the regularized inverse using RcppArmadillo
> invcpp <- HighFreq::calc_invsvd(retp, dimax=3)
> all.equal(invreg, invcpp, check.attributes=FALSE)
> # Calculate the regularized inverse from Moore-Penrose pseudo-inve
> retsq <- t(retp) %*% retp
> eigend <- eigen(retsq)
> inv2 <- eigend$vectors[, dimax] %*%
+   (t(eigend$vectors[, dimax]) / eigend$values[dimax])
> invmp <- inv2 %*% t(retp)
> all.equal(invreg, invmp, check.attributes=FALSE)
```

Linear Transformation of the Predictor Matrix

A *multivariate* linear regression model can be transformed by replacing its *predictors* x_j with their own linear combinations.

This is equivalent to multiplying the *predictor matrix* $\mathbb{X}$ by a transformation matrix $\mathbb{W}$:

$$\mathbb{X}_{trans} = \mathbb{X}\,\mathbb{W}$$

The transformed *predictor matrix* $\mathbb{X}_{trans}$ produces the same *influence matrix* $\mathbb{H}$ as the original *predictor matrix* $\mathbb{X}$:

$$\mathbb{H}_{trans} = \mathbb{X}_{trans}(\mathbb{X}_{trans}^T\mathbb{X}_{trans})^{-1}\mathbb{X}_{trans}^T =$$
$$\mathbb{X}\mathbb{W}(\mathbb{W}^T\mathbb{X}^T\mathbb{X}\mathbb{W})^{-1}\mathbb{W}^T\mathbb{X}^T =$$
$$\mathbb{X}\mathbb{W}\mathbb{W}^{-1}(\mathbb{X}^T\mathbb{X})^{-1}\mathbb{W}^{T\,-1}\mathbb{W}^T\mathbb{X}^T =$$
$$\mathbb{X}(\mathbb{X}^T\mathbb{X})^{-1}\mathbb{X}^T = \mathbb{H}$$

Since the *influence matrix* $\mathbb{H}$ is the same, the transformed regression model produces the same *fitted values* and *residuals* as the original regression model, so it's equivalent to it.

```
> # Define transformation matrix
> matv <- matrix(runif(ncols^2, min=(-1), max=1), ncol=ncols)
> # Calculate the linear combinations of predictor columns
> predt <- predm %*% matv
> # Calculate the influence matrix of the transformed predictor
> influencet <- predt %*% MASS::ginv(predt)
> # Compare the influence matrices
> all.equal(infmat, influencet)
[1] TRUE
```

Principal Component Regression

In *Principal Component Regression* (*PCR*), the predictor matrix $\mathbb{X}$ is multiplied by the *PCA rotation matrix* $\mathbb{W}$:

$$\mathbb{X}_{pca} = \mathbb{X}\mathbb{W}$$

So that the principal component vectors form the columns of the new predictor matrix.

Since the new *PCR* predictors x_i^{pca} are orthogonal, the regression coefficients are simply:

$$\beta_i = \frac{x_i^{pca} \cdot y}{\sigma_i^2}$$

Where $x_i^{pca} \cdot y$ are the inner products of the *PCR* predictors x_i^{pca} times the *response vector* y, and $\sigma_i^2 = x_i^{pca} \cdot x_i^{pca}$ are the inner products (sum of squares) of the predictors x_i^{pca}.

```
> # Perform PCA of the predictors
> pcad <- prcomp(predm, center=FALSE, scale=FALSE)
> # Calculate the PCA predictors
> predpca <- predm %*% pcad$rotation
> # Principal components are orthogonal to each other
> round(t(predpca) %*% predpca, 2)
> # Calculate the PCA influence matrix
> infmat <- predm %*% MASS::ginv(predm)
> infpca <- predpca %*% MASS::ginv(predpca)
> all.equal(infmat, infpca)
> # Calculate the regression coefficients
> coeffv <- drop(MASS::ginv(predm) %*% respv)
> # Transform the collinear regression coefficients to the PCA
> drop(coeffv %*% pcad$rotation)
> # Calculate the PCA regression coefficients
> drop(MASS::ginv(predpca) %*% respv)
> # Calculate the PCA regression coefficients directly
> colSums(predpca*drop(respv))/colSums(predpca^2)
```

Dimension Reduction Using Principal Component Regression

If the predictor columns are *collinear* then some of the *PCR* predictor squares are zero $\sigma_i^2 = 0$, and the associated regression coefficients are infinite (indeterminate) and should be discarded.

The regression can also become *singular* if the number of rows of the predictor is too small, or is even less than the number of its columns.

The regression can be *regularized* by removing the infinite or very large *PCR* regression coefficients, and transforming the coefficients back to the original predictor coordinates.

This is called *dimension reduction* - excluding the principal components with very small squares.

Dimension reduction can also be applied to reduce model overfitting by reducing the number of effective predictors.

```
> # Create almost collinear predictors
> predcol <- predm
> predcol[, 1] <- (predcol[, 1]/1e3 + predcol[, 2])
> # Calculate the collinear regression coefficients
> coeffv <- drop(MASS::ginv(predcol) %*% respv)
> coeffv
> # Calculate the PCA predictors
> pcad <- prcomp(predcol, center=FALSE, scale=FALSE)
> predpca <- predcol %*% pcad$rotation
> round(t(predpca) %*% predpca, 6)
> # Transform the collinear regression coefficients to the PCA
> drop(coeffv %*% pcad$rotation)
> # Calculate the PCA regression coefficients
> coeffpca <- drop(MASS::ginv(predpca) %*% respv)
> # Calculate the PCA regression coefficients directly
> colSums(predpca*drop(respv))/colSums(predpca^2)
> # Transform the PCA regression coefficients to the original coordi
> drop(coeffpca %*% MASS::ginv(pcad$rotation))
> coeffv
> # Calculate the regression coefficients after dimension reduction
> npca <- NROW(coeffpca)
> drop(coeffpca[-npca] %*% MASS::ginv(pcad$rotation)[-npca, ])
> # Compare with the collinear regression coefficients
> coeffv
> # Calculate the original regression coefficients
> drop(MASS::ginv(predm) %*% respv)
```

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.

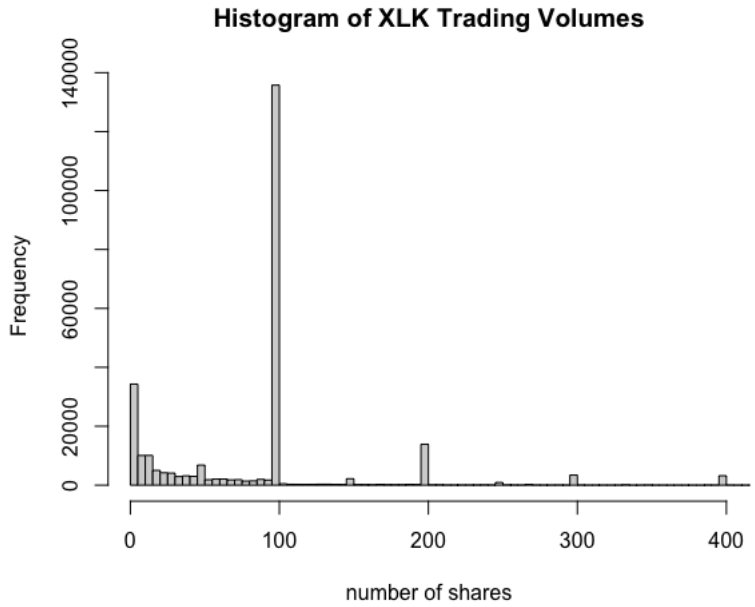
```
> library(HighFreq)
> # Read TAQ trade data from csv file
> taq <- data.table::fread(file="/Users/jerzy/Develop/data/xlk_tick_
> # Inspect the TAQ data in data.table format
> taq
> class(taq)
> colnames(taq)
> sapply(taq, class)
> symbol <- taq$SYM_ROOT[1]
> # Create date-time index
> datev <- paste(taq$DATE,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

Trading Volumes in High Frequency Data

The trading volumes represent the number of shares traded at a given price.

The histogram of the trading volumes shows that the highest frequencies of trades are for 100 shares and for round lots (trades that are multiples of 100 shares.)

There are also significant frequencies for *odd lots*, with small volumes of less than 100 shares.




```
> # Coerce trade ticks to xts series
> xlk <- xts::xts(taq[, .(price, volume)], datev)
> colnames(xlk) <- c("price", "volume")
> save(xlk, file="/Users/jerzy/Develop/data/xlk_tick_trades2020_0316
> # save(xlk, file="/Users/jerzy/Develop/data/xlk_tick_trades2020_03
> # Plot histogram of the trading volumes
> hist(xlk$volume, main="Histogram of XLK Trading Volumes",
+      breaks=1e5, xlim=c(1, 400), xlab="number of shares")
```

Microstructure Noise in High Frequency Data

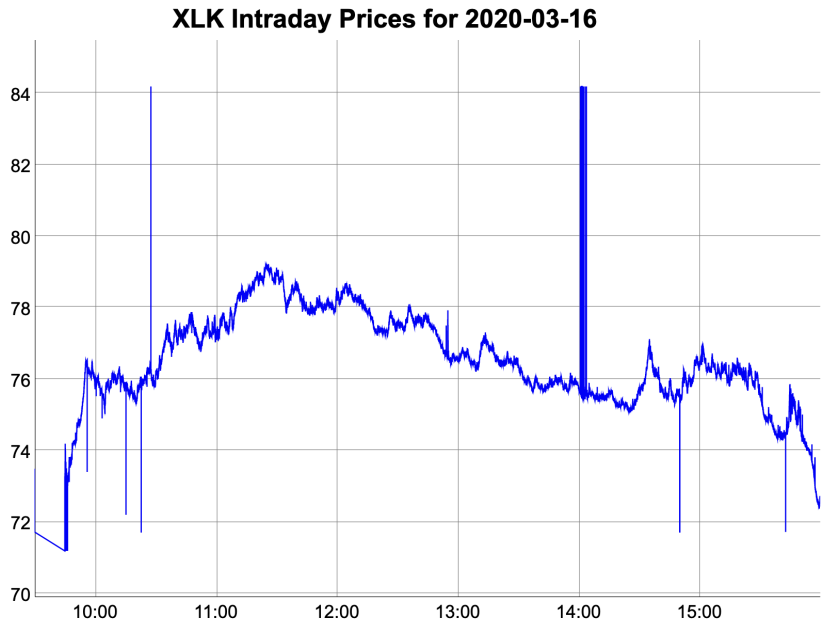
High frequency data contains *microstructure noise* in the form of *price spikes* and the *bid-ask bounce*.

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

Price spikes are often caused by data collection errors, but sometimes they represent actual trades with very large lot (trade) sizes.

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 reality the mid price is unchanged.




```
> # Plot dygraph
> dygraphs::dygraph(xlk$price, main="XLK Intraday Prices for 2020-03
+   dyOptions(colors="blue", strokeWidth=1)
> # Plot in x11 window
> x11(width=6, height=5)
> quantmod::chart_Series(x=xlk$price, name="XLK Intraday Prices for
```

Microstructure Noise And Trading Volumes in High Frequency Data

The number of the *price spikes* depends on the level of trading volumes, with the number decreasing with higher trading volumes.


```
> # Plot dygraph of trade prices of at least 100 shares
> dygraphs::dygraph(xlk$price[xlk$volume >= 100, ],
+   main="XLK Prices for Trades of At Least 100 Shares") %>%
+   dyOptions(colors="blue", strokeWidth=1)
```

Filtering Microstructure Noise From High Frequency Data

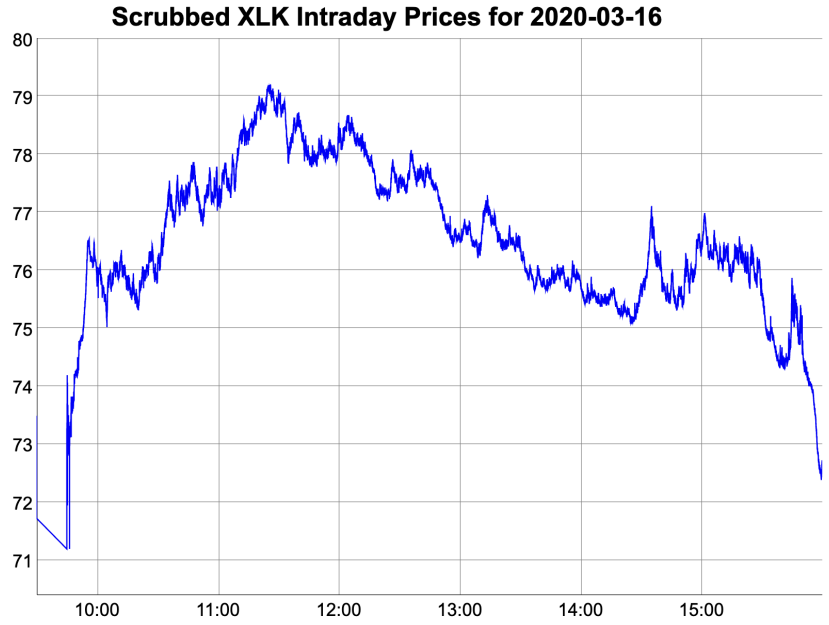
Microstructure noise in high frequency data can be identified using a *Hampel filter*.

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

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

If the absolute value of the *z-score* exceeds the *threshold value* then it's classified as *bad data*, and it can be removed or replaced.

```
> # Calculate the centered Hampel filter to remove bad prices
> lookb <- 71
> half_back <- lookb %/% 2
> pricev <- xlk$price
> # Calculate the trailing median and MAD
> medianv <- HighFreq::roll_mean(pricev, lookb=lookb, method="nonpa
> colnames(medianv) <- c("median")
> madv <- HighFreq::roll_var(pricev, lookb=lookb, method="nonparame
> # madv <- TTR::runMAD(pricev, n=lookb)
> # Center the median and the MAD
> medianv <- rutils::lagit(medianv, lagg=(-half_back), pad_zeros=FA
> madv <- rutils::lagit(madv, lagg=(-half_back), pad_zeros=FALSE)
> # Calculate the Z-scores
> zscores <- ifelse(madv > 0, (pricev - medianv)/madv, 0)
> # Z-scores have very fat tails
> range(zscores); mad(zscores)
> madz <- mad(zscores[abs(zscores) > 0])
> hist(zscores, breaks=50000, xlim=c(-2*madz, 2*madz))
```




```
> # Define discrimination threshold value
> threshv <- 6*madz
> # Identify good prices with small z-scores
> isgood <- (abs(zscores) < threshv)
> # Calculate the number of bad prices
> sum(!isgood)
> # Overwrite bad prices and calculate time series of scrubbed price
> priceg <- pricev
> priceg[!isgood] <- NA
> priceg <- na.locf(priceg)
> # Plot dygraph of the scrubbed prices
> dygraphs::dygraph(priceg, main="Scrubbed XLK Intraday Prices") %>%
+   dyOptions(colors="blue", strokeWidth=1)
> # Plot using chart_Series()
> x11(width=6, height=5)
> quantmod::chart_Series(x=priceg,
+   name="Clean XLK Intraday Prices for 2020-03-16")
```

Classifying Data Outliers Using the Hampel Filter

The Hampel filter is a *classifier* which classifies the prices as either good or bad data points.

In order to measure the performance of the Hampel filter, we add price spikes to the clean prices, to see how accurately they're classified.

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.

```
> # Add 200 random price spikes to the clean prices
> set.seed(1121, "Mersenne-Twister", sample.kind="Rejection")
> nspikes <- 200
> nrows <- NROW(priceg)
> ispike <- logical(nrows)
> ispike[sample(x=nrows, size=nspikes)] <- TRUE
> priceb <- priceg
> priceb[ispike] <- priceb[ispike]*
+   sample(c(0.999, 1.001), size=nspikes, replace=TRUE)
> # Calculate the z-scores
> medianv <- HighFreq::roll_mean(priceb, lookb=lookb, method="nonpar
> # Plot the bad prices and their medians
> pricem <- cbind(priceb, medianv)
> colnames(pricem) <- c("prices with spikes", "median")
> dygraphs::dygraph(pricem, main="XLK Prices With Spikes") %>%
+   dyOptions(colors=c("red", "blue"))
> # medianv <- TTR::runMedian(priceb, n=lookb)
> madv <- HighFreq::roll_var(priceb, lookb=lookb, method="nonparamet
> # madv <- TTR::runMAD(priceb, n=lookb)
> zscores <- ifelse(madv > 0, (priceb - medianv)/madv, 0)
> # Z-scores have very fat tails
> range(zscores); mad(zscores)
> madz <- mad(zscores[abs(zscores) > 0])
> hist(zscores, breaks=10000, xlim=c(-4*madz, 4*madz))
> # Identify good prices with small z-scores
> threshv <- 3*madz
> isgood <- (abs(zscores) < threshv)
> sum(!isgood)
```

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.

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

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

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).

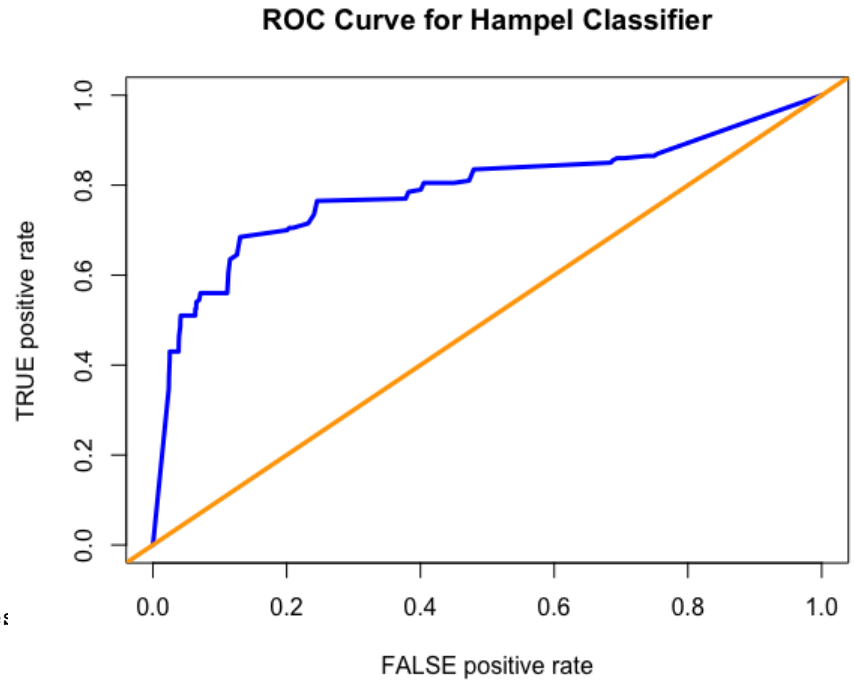
The sum of the *true negative* plus the *false positive* rate is equal to 1.

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, threshv) {
+     confmat <- table(actualv, (abs(zscores) < threshv))
+     confmat <- confmat / rowSums(confmat)
+     c(typeI=confmat[2, 1], typeII=confmat[1, 2])
+ }  # end confun
> confun(!ispike, zscores, threshv=threshv)
> # Define vector of discrimination thresholds
> threshv <- madz*seq(from=0.1, to=5.0, by=0.1)/2
> # Calculate the error rates
> errorr <- sapply(threshv, confun, actualv=!ispike, zscores=zscores
> errorr <- t(errorr)
> rownames(errorr) <- threshv
> errorr <- rbind(c(1, 0), errorr)
> errorr <- rbind(errorr, c(0, 1))
> # Calculate the area under the ROC curve (AUC)
> truepos <- (1 - errorr[, "typeII"])
> truepos <- (truepos + rutils::lagit(truepos))/2
> falsepos <- rutils::diffit(errorr[, "typeI"])
> abs(sum(truepos*falsepos))
```



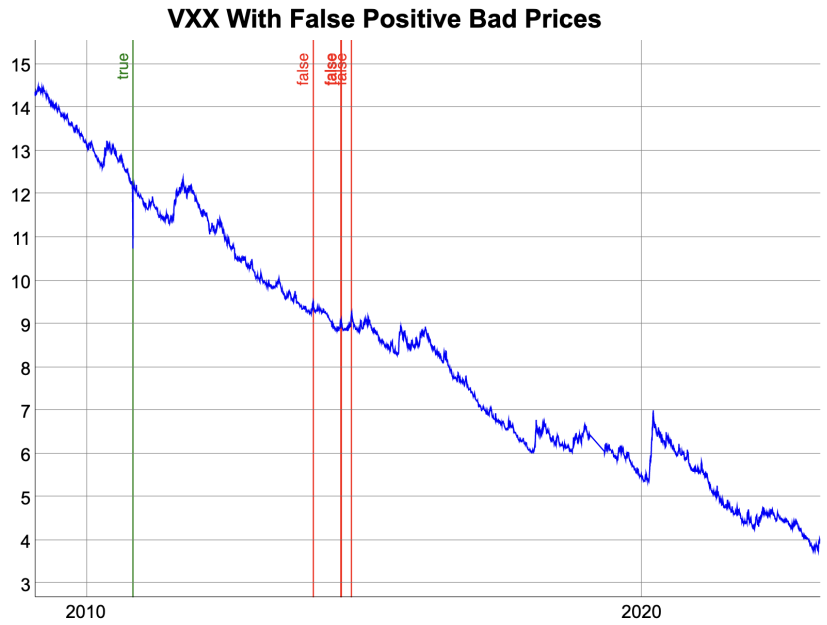

```
> # Plot ROC curve for Hampel classifier
> plot(x=errorr[, "typeI"], y=1-errorr[, "typeII"],
+      xlab="FALSE positive rate", ylab="TRUE positive rate",
+      xlim=c(0, 1), ylim=c(0, 1),
+      main="ROC Curve for Hampel Classifier",
+      type="l", lwd=3, col="blue")
> abline(a=0.0, b=1.0, lwd=3,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

Filtering Bad Data From Daily Stock Prices

Daily stock prices also contain bad data points consisting of mostly single, isolated spikes in prices.

The number of false positives may be too high, so the Hampel filter parameters (the look-back interval and the threshold) need adjustment.

For example, the *VXX* has only one bad price (on 2010-11-08), but the Hampel filter identifies many more than that (which are false positives).




```
> # Calculate the centered Hampel filter for VXX
> lookb <- 71
> half_back <- lookb %/% 2
> pricev <- log(na.omit(rutils::etfenv$prices$VXX))
> medianv <- roll::roll_median(pricev, width=lookb)
> medianv[1:lookb, ] <- pricev[1:lookb, ]
> medianv <- rutils::lagit(medianv, lagg=(-half_back), pad_zeros=FA
> madv <- HighFreq::roll_var(pricev, lookb=lookb, method="nonparam
> madv <- rutils::lagit(madv, lagg=(-half_back), pad_zeros=FALSE)
> zscores <- ifelse(madv > 0, (pricev - medianv)/madv, 0)
> range(zscores); mad(zscores)
> madz <- mad(zscores[abs(zscores) > 0])
> hist(zscores, breaks=100, xlim=c(-3*madz, 3*madz))
```

```
> # Define discrimination threshold value
> threshv <- 10*madz
> # Calculate the bad prices
> isgood <- (abs(zscores) < threshv)
> sum(!isgood)
> # Dates of the bad prices
> zoo::index(pricev[!isgood])
> # Calculate the false positives
> falsep <- !isgood
> falsep[which(zoo::index(pricev) == as.Date("2010-11-08"))] <- FALS
> # Plot dygraph of the prices with bad prices
> dygraphs::dygraph(pricev, main="VXX Prices With False Positives")
+   dyEvent(zoo::index(pricev[falsep]), label=rep("false", sum(false
+   dyEvent(zoo::index(pricev["2010-11-08"]), label="true", strokePa
+   dyOptions(colors="blue", strokeWidth=1)
```

draft: Filtering Combined Spikes From Stock Prices

The narrow Hampel filter isn't very good anyway

The narrow Hampel filter using the median of 3 prices can only identify single isolated spikes.

But sometimes several bad prices occur in a row, one after another.

The narrow Hampel filter cannot identify multiple bad prices in a row, and will therefore produce false negatives (bad prices identified as good).

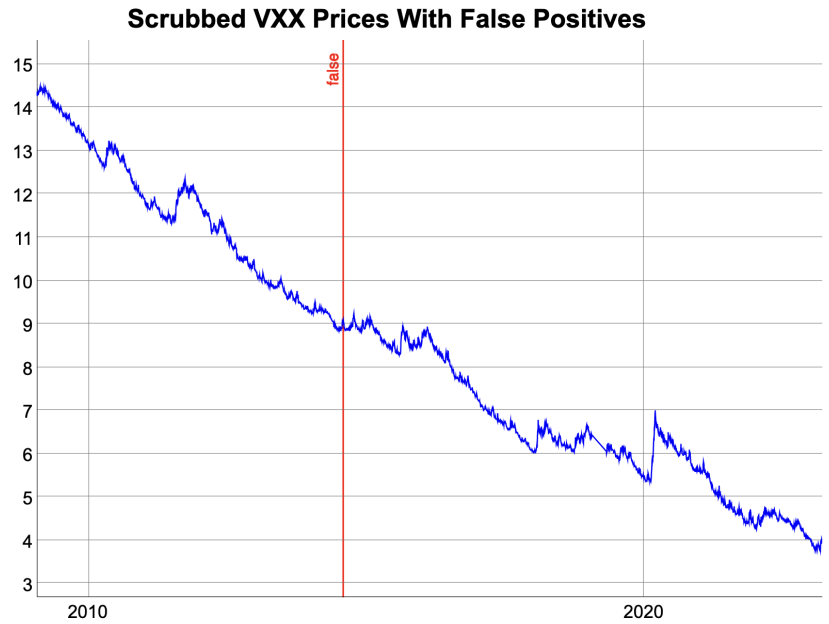
```
> # Add single isolated spike to the prices
> priceb <- pricev
> priceb["2017-11-20"] <- 1.2*priceb["2017-11-20"]
> # Calculate the Z-scores
> medianv <- roll::roll_median(priceb, width=lookb)
> medianv[1:lookb, ] <- priceb[1:lookb, ]
> medianv <- rutils::lagit(medianv, lagg=(-half_back), pad_zeros=FAI
> madv <- HighFreq::roll_var(priceb, lookb=lookb, method="nonparamet
> madv <- rutils::lagit(madv, lagg=(-half_back), pad_zeros=FALSE)
> zscores <- ifelse(madv > 0, (priceb - medianv)/madv, 0)
> madz <- mad(zscores[abs(zscores) > 0])
> # Calculate the number of bad prices
> threshv <- 10*madz
> isgood <- (abs(zscores) < threshv)
> sum(!isgood)
> zoo::index(priceb[!isgood])
> # Add two neighboring spikes to the prices
> priceb <- pricev
> priceb["2017-11-20"] <- 1.2*priceb["2017-11-21"]
> priceb["2017-11-21"] <- 1.2*priceb["2017-11-21"]
> # Calculate the Z-scores
> medianv <- roll::roll_median(priceb, width=lookb)
> medianv[1:lookb, ] <- priceb[1:lookb, ]
> medianv <- rutils::lagit(medianv, lagg=(-half_back), pad_zeros=FAI
> madv <- HighFreq::roll_var(priceb, lookb=lookb, method="nonparamet
> madv <- rutils::lagit(madv, lagg=(-half_back), pad_zeros=FALSE)
> zscores <- ifelse(madv > 0, (priceb - medianv)/madv, 0)
> madz <- mad(zscores[abs(zscores) > 0])
> # Calculate the number of bad prices
> isgood <- (abs(zscores) < threshv)
> sum(!isgood)
> zoo::index(priceb[!isgood])
```

Scrubbing Bad Stock Prices

Bad stock prices can be scrubbed (replaced) with the previous good price.

But it's incorrect to replace bad prices with the average of the previous good price and the next good price, since that would cause data snooping.

```
> # Dates of the bad prices
> datev <- zoo::index(pricev)
> dateb <- datev[!isgood]
> # Dates of the previous prices
> datep <- c(!isgood[-1], FALSE)
> datev[datep]
> # Replace bad stock prices with the previous good prices
> priceg <- pricev
> priceg[!isgood] <- pricev[datep]
> # Calculate the Z-scores
> medianv <- roll::roll_median(priceg, width=lookb)
> medianv[1:lookb, ] <- priceg[1:lookb, ]
> medianv <- rutils::lagit(medianv, lagg=(-half_back), pad_zeros=FA
> madv <- HighFreq::roll_var(priceg, lookb=lookb, method="nonparame
> madv <- rutils::lagit(madv, lagg=(-half_back), pad_zeros=FALSE)
> zscores <- ifelse(madv > 0, (priceg - medianv)/madv, 0)
> madz <- mad(zscores[abs(zscores) > 0])
> # Calculate the number of bad prices
> threshv <- 10*madz
> isgood <- (abs(zscores) < threshv)
> sum(!isgood)
> zoo::index(priceg[!isgood])
```




```
> # Calculate the false positives
> falsep <- !isgood
> falsep[which(zoo::index(pricev) == as.Date("2010-11-08"))] <- FALS
> # Plot dygraph of the prices with bad prices
> dygraphs::dygraph(priceg, main="Scrubbed VXX Prices With False Pos
+   dyEvent(zoo::index(priceg[falsep]), label=rep("false", sum(false
+   dyOptions(colors="blue", strokeWidth=1)
```

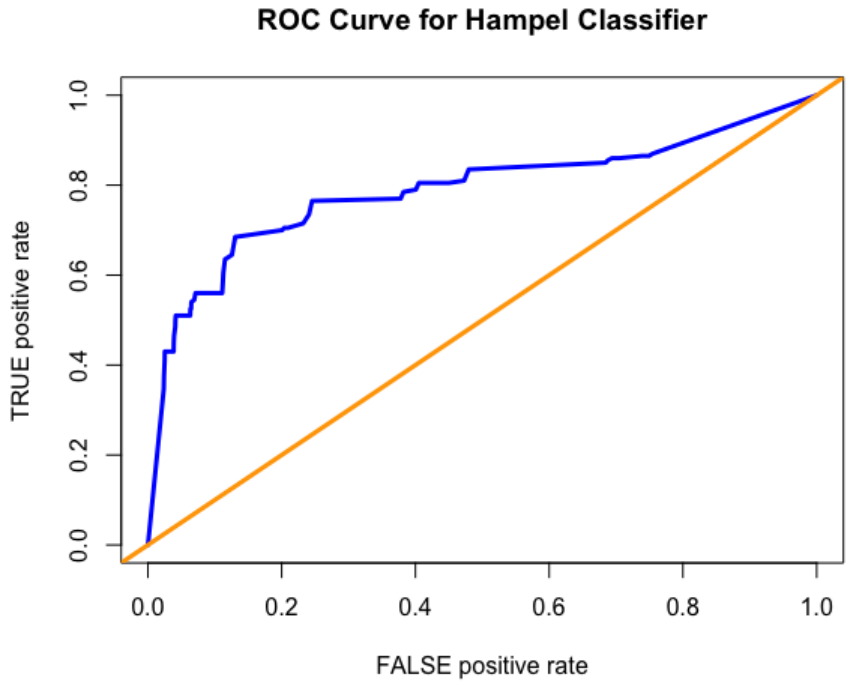
draft: Receiver Operating Characteristic (ROC) Curve

The performance of the Hampel noise classification model depends on the length of the look-back time interval. a binary. *area under the ROC curve* (AUC) is a measure of a binary. The optimal *threshold value* can be determined using *cross-validation*.

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




```
> # Plot ROC curve for Hampel classifier
> x11(width=6, height=5)
> plot(x=errorr[, "typeI"], y=1-errorr[, "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")
```

The *Logistic* Function

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

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

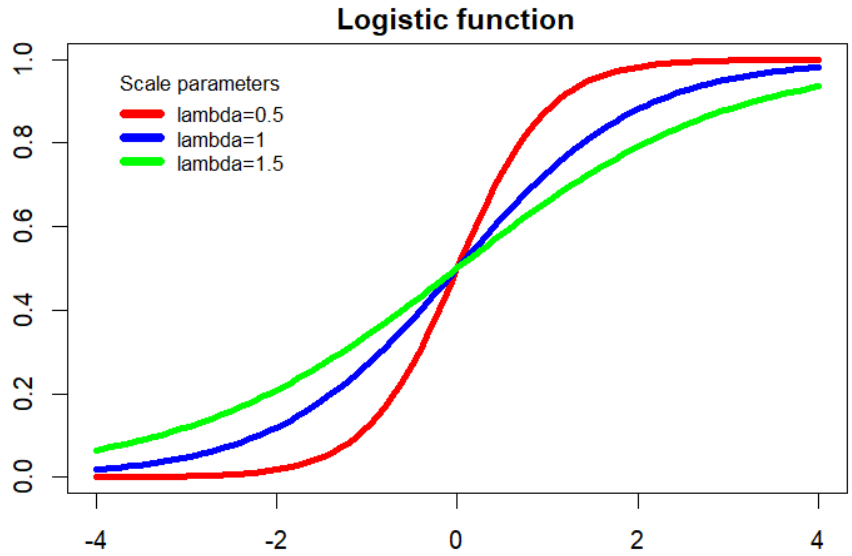
Where λ is the scale (dispersion) parameter.

The *logistic* function is often used as an activation function in neural networks, and logistic regression can be viewed as a perceptron (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,




```
> lambdav <- 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=lambdav[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", lambdav, sep="="), y.intersp=0.4,
+        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.

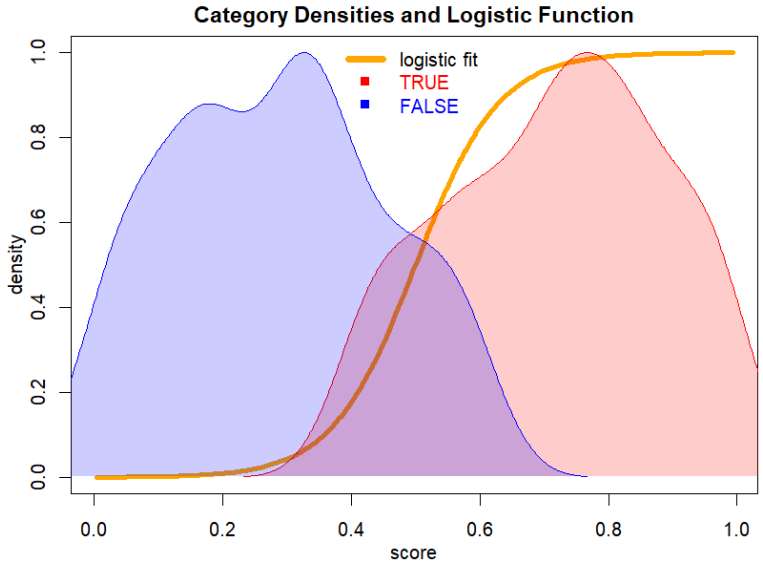
The function `glm()` fits generalized linear models, including *logistic* regressions.

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.

```
> # Initialize the random number generator
> set.seed(1121, "Mersenne-Twister", sample.kind="Rejection")
> # 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
> predm <- c(sample1, sample2)
> respv <- c(logical(100), !logical(100))
> # Perform logit regression
> logmod <- glm(respv ~ predm, family=binomial(logit))
> class(logmod)
> summary(logmod)
```




```
> ordern <- order(predm)
> plot(x=predm[ordern], y=logmod$fitted.values[ordern],
+      main="Category Densities and Logistic Function",
+      type="l", lwd=4, col="orange", xlab="predictor", ylab="densit
> densv <- density(predm[respv])
> densv$y <- densv$y/max(densv$y)
> lines(densv, col="red")
> polygon(c(min(densv$x), densv$x, max(densv$x)), c(min(densv$y), de
> densv <- density(predm[!respv])
> densv$y <- densv$y/max(densv$y)
> lines(densv, col="blue")
> polygon(c(min(densv$x), densv$x, max(densv$x)), c(min(densv$y), de
> # 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), y.intersp=0.4,
+  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 $(1 - p)$.

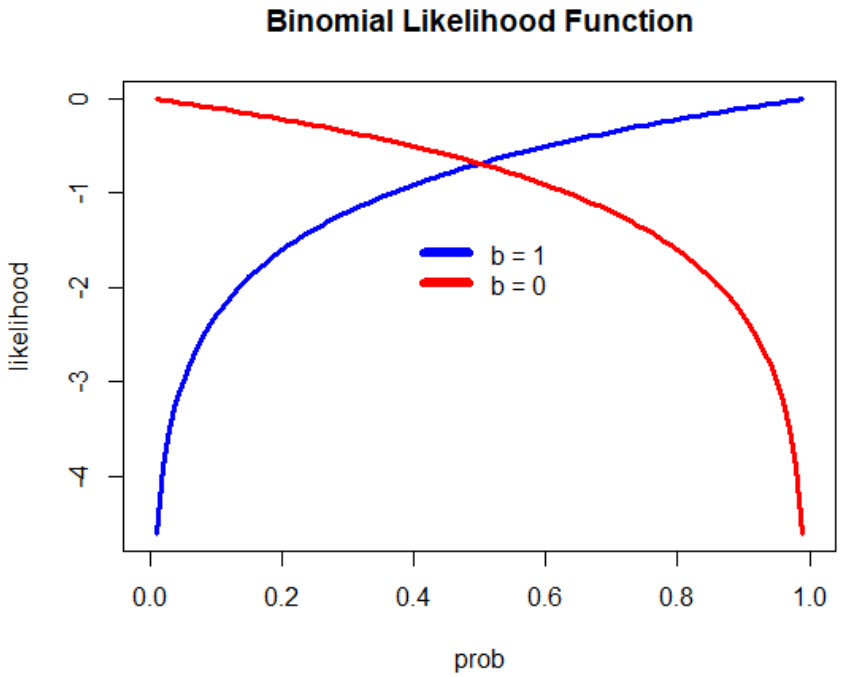
Then b follows the binomial distribution:

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

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=0.4,
+        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.

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

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(vecv, param=25) {
+   sum(vecv^2 - param*cos(vecv))
+ }  # end rastrigin
> vecv <- c(pi/6, pi/6)
> rastrigin(vecv=vecv)
> # Draw 3d surface plot of Rastrigin function
> options(rgl.useNULL=TRUE); library(rgl)
> rgl::persp3d(
+   x=Vectorize(function(x, y) rastrigin(vecv=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=vecv, 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
> optiml <- optim(par=initp,
+         fn=likefun, # Log-likelihood function
+         method="L-BFGS-B", # Quasi-Newton method
+         respv=respv,
+         predm=predm,
+         upper=c(20, 20), # Upper constraint
+         lower=c(-20, -20), # Lower constraint
+         hessian=TRUE)
> # Optimal logistic parameters
> optiml$par
> unname(logmod$coefficients)
> # Standard errors of parameters
> sqrt(diag(solve(optiml$hessian)))
> regsum <- summary(logmod)
> regsum$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()`.

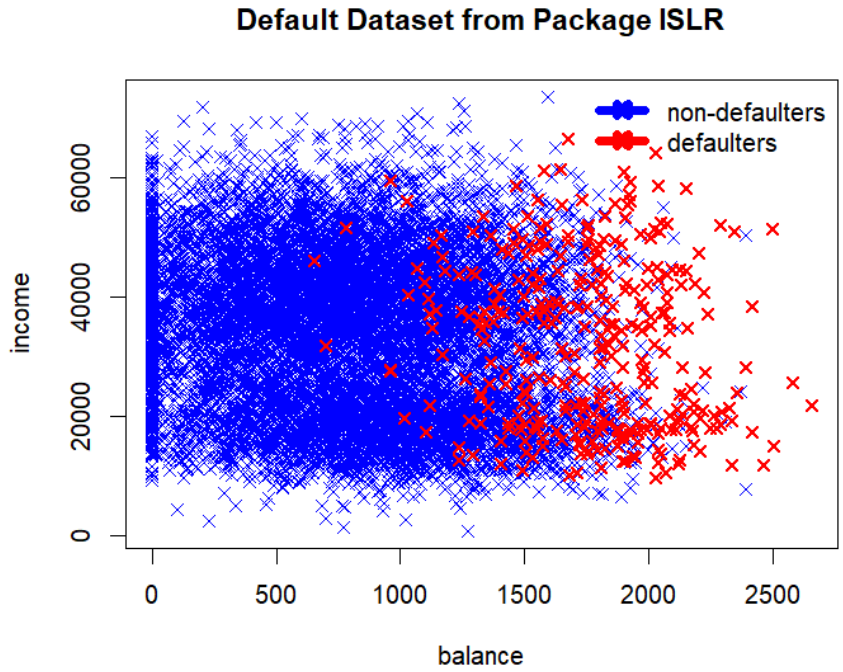
```
> # Coerce the default and student columns to Boolean
> Default <- ISLR::Default
> Default$default <- (Default$default == "Yes")
> Default$student <- (Default$student == "Yes")
> colnames(Default)[1:2] <- c("default", "student")
> attach(Default)  # Attach Default to search path
> # Explore credit 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=0.4, bty="n", col=c("blue", "red"), lty=1, lwd=6, pch=4
```

Boxplots of the Default Dataset

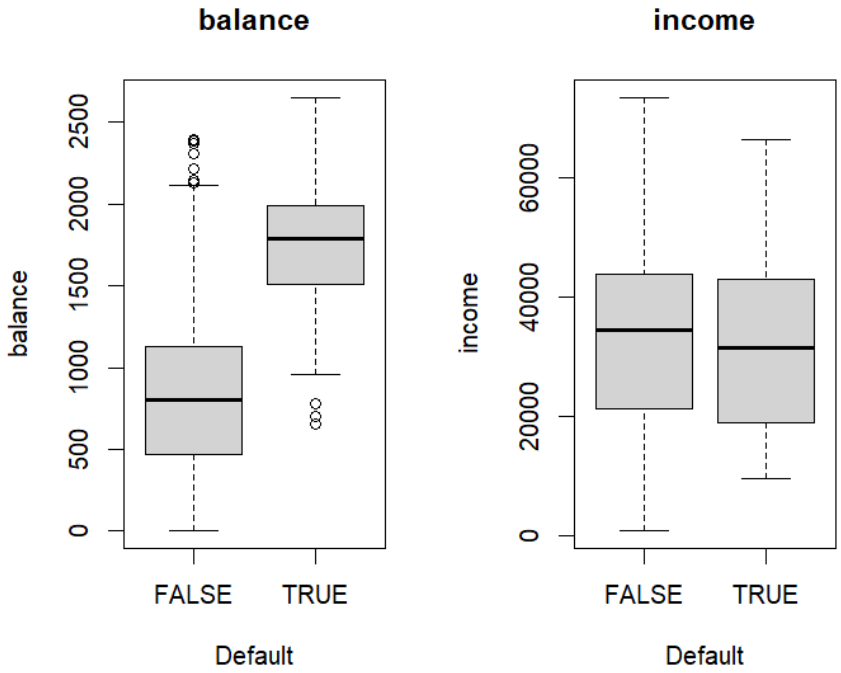
A *Box Plot* (box-and-whisker plot) is a graphical display of a distribution of data:

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")
```

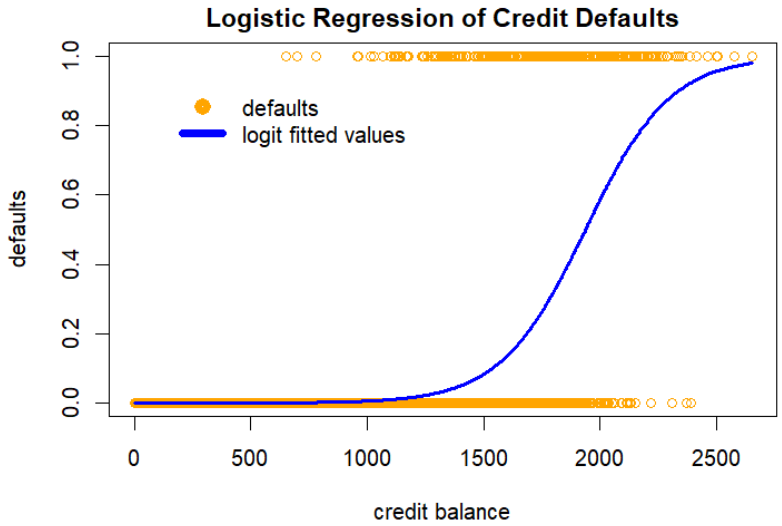
Modeling Credit Defaults Using *Logistic* Regression

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))

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

Number of Fisher Scoring iterations: 8
```



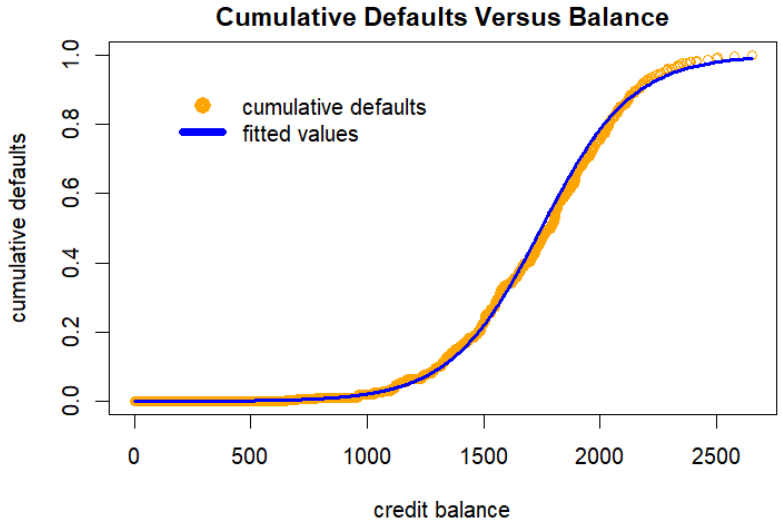

```
> x11(width=6, height=5)
> par(mar=c(4, 4, 2, 2), oma=c(0, 0, 0, 0), mgp=c(2.5, 1, 0))
> plot(x=balance, y=default,
+      main="Logistic Regression of Credit Defaults",
+      col="orange", xlab="credit balance", ylab="defaults")
> ordern <- order(balance)
> lines(x=balance[ordern], y=logmod$fitted.values[ordern], col="blue
> legend(x="topleft", inset=0.1, bty="n", lwd=6, y.intersp=0.4,
+  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 the cumulative defaults
> sumd <- sum(default)
> defaultv <- sapply(balance, function(balv) {
+     sum(default[balance <= balv])
+ })  # 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=0.4,
+  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)

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.

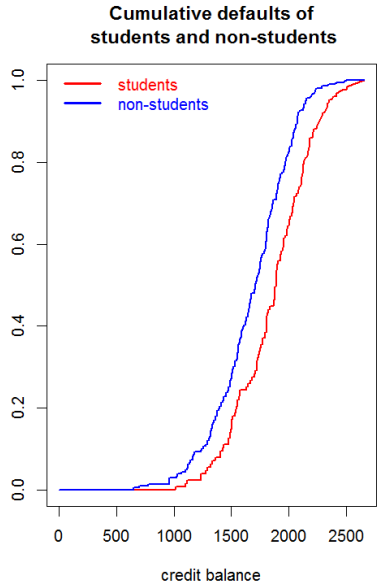
But the coefficient from the single-factor regression is positive (indicating that students are more likely to default), while the coefficient from the multifactor regression is negative (indicating that students are less likely to default).

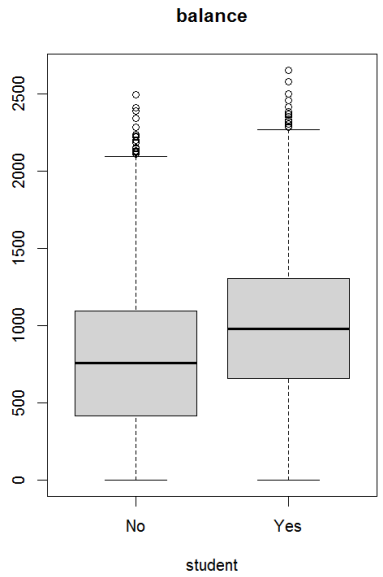
The reason that students are more likely to default is because they have higher credit balances than non-students - which is what the single-factor regression shows.

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
```

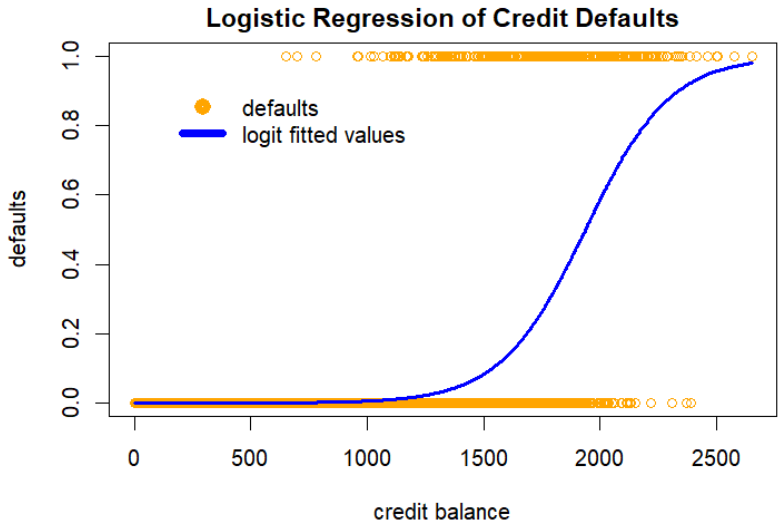
```
> # Calculate the cumulative defaults
> cum_defaults <- sapply(balance, function(balv) {
+ c(student=sum(default[student & (balance <= balv)]),
+   non_student=sum(default[!student & (balance <= balv)]))
+ })  # end sapply
> total_defaults <- c(student=sum(student & default),
+       student=sum(!student & 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", lw
> legend(x="topleft", bty="n", y.intersp=0.4,
+  legend=c("students", "non-students"),
+  col=c("red", "blue"), text.col=c("red", "blue"), lwd=3)
> # Balance boxplot for student factor
```

draft: Modeling Credit Defaults Using Student Status

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

Persons who are students are more likely to default because students have higher credit balances.

```
> # Fit logistic regression model
> logmod <- glm(default ~ student, family=binomial(logit))
> summary(logmod)
```




```
> x11(width=6, height=5)
> par(mfrow=c(1,2))  # Set plot panels
> # Balance boxplot
> boxplot(formula=balance ~ default,
+   col="lightgrey", main="balance", xlab="Default")
>
>
> # Plot data points for non-students
> x11(width=6, height=5)
> 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[!student, ])
> # Plot data points for students
> points(income ~ balance, pch=4, lwd=2, col="red",
+  data=Default[student, ])
> # Add legend
> legend(x="topright", bty="n", y.intersp=0.4,
+  legend=c("non-students", "students"),
+  col=c("blue", "red"), lty=1, lwd=6, pch=4)
```

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
> fcast <- predict(logmod, type="response")
> all.equal(logmod$fitted.values, fcast)
[1] TRUE
> # Define discrimination threshold value
> threshv <- 0.7
> # Calculate the confusion matrix in-sample
> table(actual=!default, forecast=(fcast < threshv))
       forecast
actual  FALSE TRUE
  FALSE    57  276
  TRUE     12 9655
> # Fit logistic regression over training data
> # Initialize the random number generator
> set.seed(1121, "Mersenne-Twister", sample.kind="Rejection")
> nrows <- NROW(Default)
> samplev <- sample.int(n=nrows, size=nrows/2)
> trainset <- Default[samplev, ]
> logmod <- glm(formulav, data=trainset, family=binomial(logit))
> # Forecast over test data out-of-sample
> testset <- Default[-samplev, ]
> fcast <- predict(logmod, newdata=testset, type="response")
> # Calculate the confusion matrix out-of-sample
> table(actual=!testset$default, forecast=(fcast < threshv))
       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 the confusion matrix out-of-sample
> confmat <- table(actual=!testset$default,
+ forecast=(fcast < threshv))
> confmat
       forecast
actual  FALSE TRUE
  FALSE    29  132
  TRUE      9 4830
> # Calculate the FALSE positive (type I error)
> sum(!testset$default & (fcast < threshv))
[1] 4830
> # Calculate the FALSE negative (type II error)
> sum(testset$default & (fcast > threshv))
[1] 29
```

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 the 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).

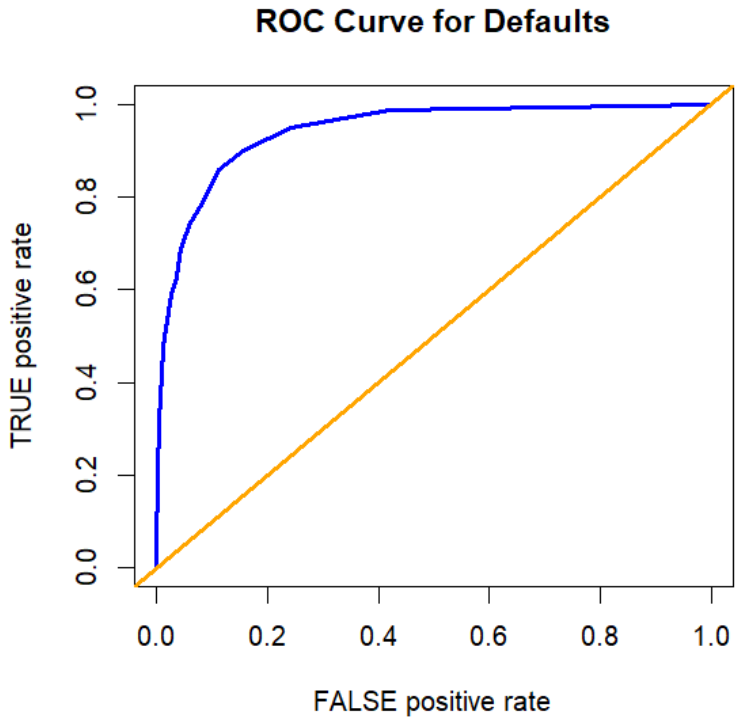
The sum of the *true negative* plus the *false positive* rate is equal to 1.

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




```
> # Plot ROC Curve for Defaults
> x11(width=5, height=5)
> plot(x=errorr[, "typeI"], y=1-errorr[, "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")
```

draft: State Space Models

A *state space model* is a stochastic process for a *state variable* θ, which is subject to *measurement error*.

The *state variable* θ is latent (not directly observable), and its value is only measured by observing the *measurement variable* y_t.

A simple *state space model* can be written as a *transition equation* and a *measurement equation*:

$$\theta_t = g_t \theta_{t-1} + w_t$$
$$y_t = f_t \theta_t + v_t$$

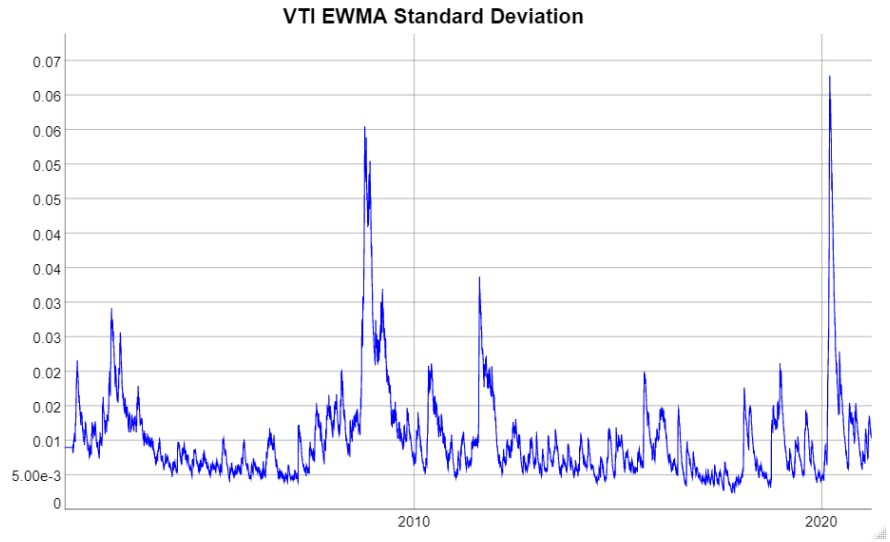
Where w_t and v_t follow the normal distributions $\phi(0, \sigma_t^w)$ and $\phi(0, \sigma_t^v)$.

The system variables (matrices) g_t and f_t are deterministic functions of time.

If the *time series* has zero *expected* mean, then the *EMA realized* variance estimator can be written approxiamtely as: σ_t^2 is the weighted *realized* variance, equal to the weighted average of the point realized variance for period `i` and the past *realized* variance.

The parameter λ determines the rate of decay of the *EMA* weights, with smaller values of λ producing faster decay, giving more weight to recent realized variance, and vice versa.

The function `stats:::C_cfilter()` calculates the convolution of a vector or a time series with a filter of coefficients (weights).




```
> # Calculate the EMA VTI variance using compiled C++ function
> lookb <- 51
> weightv <- exp(-0.1*1:lookb)
> weightv <- weightv/sum(weightv)
> varv <- .Call(stats:::C_cfilter, retp^2, filter=weightv, sides=1,
> varv[1:(lookb-1)] <- varv[lookb]
> # Plot EMA volatility
> varv <- xts:::xts(sqrt(varv), order.by=zoo::index(retp))
> dygraphs::dygraph(varv, main="VTI EMA Volatility")
> quantmod::chart_Series(varv, name="VTI EMA Volatility")
```

State Space Models

Consider a price process p_t which follows a *Brownian Motion*:

$$p_t = p_{t-1} + \eta_t$$

This equation is called the *transition* (state) equation, and it describes the time evolution of the unobservable state variable p_t.

We can only observe (measure) the value of p_t approximately due to the noise ϵ_t:

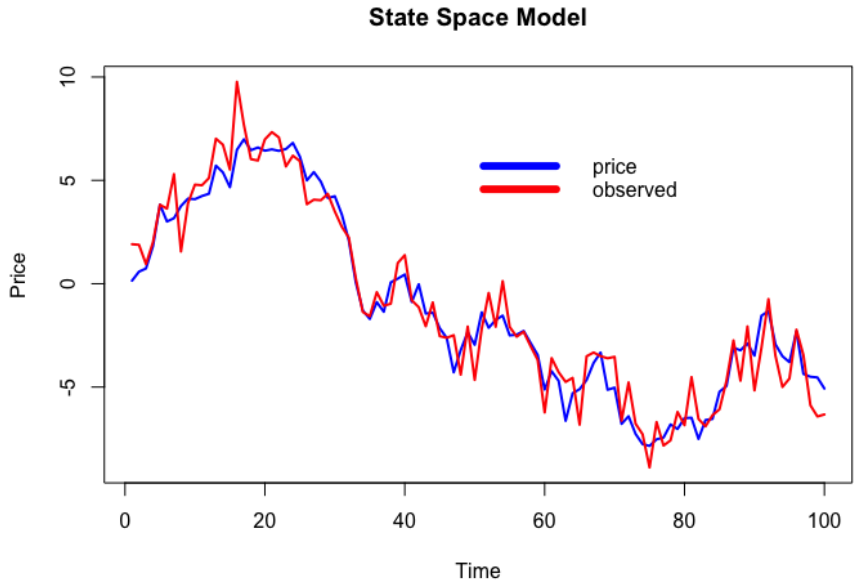
$$o_t = p_t + \epsilon_t$$

This equation is called the *measurement* equation, and it describes the observed measurement variable o_t.

The innovations ϵ_t and η_t follow *Normal* distributions with standard deviations equal to σ_ϵ and σ_η

The above two equations define a very simple *state space* model called a *level model*.

More sophisticated state space models can have more complex transition equations, but they all have similar measurement equations, where the observed values o_t are equal to the sum of the unobservable state variable p_t plus a noise ϵ_t.




```
> # Define Brownian motion prices
> # Initialize the random number generator
> set.seed(1121, "Mersenne-Twister", sample.kind="Rejection")
> nrows <- 100
> pricev <- cumsum(rnorm(nrows))
> # Calculate the observed values
> prico <- pricev + rnorm(nrows)
> # Plot the state space model
> pricev <- cbind(pricev, prico)
> colnames(pricev) <- c("price", "observed")
> matplot(y=pricev, main="State Space Model",
+   xlab="Time", ylab="Price",
+   type="l", lty="solid", lwd=2, col=c("blue", "red"))
> legend(x="topright", legend=colnames(pricev),
+  inset=0.1, cex=1.0, bg="white", bty="n", y.intersp=0.4,
+  lwd=6, lty=1, col=c("blue", "red"))
```

The Kalman Filter

Let $\hat{p}_t$ be the estimate of the price, let $\bar{p}_t$ be the expected value of the estimate, and let σ_t^2 be its variance.

The expected value $\hat{p}_t$ is the best estimate of the price $\bar{p}_t$.

Let o_t be the observed price today.

The probability distribution of the price estimate $\hat{p}_t$, conditional on $\hat{p}_{t-1}$ and on o_t, is the product of two *Standard* distributions centered on $\bar{p}_{t-1}$ and o_t:

$$\phi(\hat{p}_t|\bar{p}_{t-1}, o_t) \propto$$

$$\exp(\frac{-(\hat{p}_t - o_t)^2}{2\sigma_\epsilon^2}) \exp(\frac{-(\hat{p}_t - \bar{p}_{t-1})^2}{2(\sigma_{t-1}^2 + \sigma_\eta^2)}) \propto$$

$$\exp(\frac{-(\hat{p}_t - \bar{p}_t)^2}{2\sigma_t^2})$$

We can interpret this expression as a *likelihood function* for the expected value $\bar{p}_t$ of the estimate $\hat{p}_t$.

The expected value $\bar{p}_t$ of the estimate $\hat{p}_t$ is given by:

$$\bar{p}_t = \frac{\bar{p}_{t-1}\sigma_\epsilon^2 + o_t(\sigma_{t-1}^2 + \sigma_\eta^2)}{\sigma_\eta^2 + \sigma_\epsilon^2 + \sigma_{t-1}^2} =$$

$$\bar{p}_{t-1} + k_{t-1}(o_t - \bar{p}_{t-1})$$

Where σ_t^2 is the updated variance of $\hat{p}_t$ given by:

$$\sigma_t^2 = \frac{\sigma_\epsilon^2(\sigma_{t-1}^2 + \sigma_\eta^2)}{\sigma_{t-1}^2 + \sigma_\eta^2 + \sigma_\epsilon^2} = (1 - k_{t-1})(\sigma_{t-1}^2 + \sigma_\eta^2)$$

The ratio:

$$k_t = \frac{\sigma_t^2 + \sigma_\eta^2}{\sigma_t^2 + \sigma_\eta^2 + \sigma_\epsilon^2}$$

Is called the *Kalman gain*.

The above equations can be combined to form the *update equations*:

$$\bar{p}_t = \bar{p}_{t-1} + k_{t-1}(o_t - \bar{p}_{t-1})$$

$$\sigma_t^2 = (1 - k_{t-1})(\sigma_{t-1}^2 + \sigma_\eta^2)$$

$$k_t = \frac{\sigma_t^2 + \sigma_\eta^2}{\sigma_t^2 + \sigma_\eta^2 + \sigma_\epsilon^2}$$

The update equations allow to *recursively update* the expected value $\bar{p}_t$ and the variance σ_t^2 based on the past value $\bar{p}_{t-1}$ and the observed price o_t.

Steady State of the Kalman Filter

In the long run, the Kalman filter settles into a steady state, with the estimate variance and the Kalman gain becoming constant: $\sigma_t^2 = \sigma^2$ and $k_t = k$.

Then the update equations simplify to:

$$\sigma^2 = (1 - k)(\sigma^2 + \sigma_\eta^2)$$

$$k = \frac{\sigma^2 + \sigma_\eta^2}{\sigma^2 + \sigma_\eta^2 + \sigma_\epsilon^2}$$

Which can be transformed to:

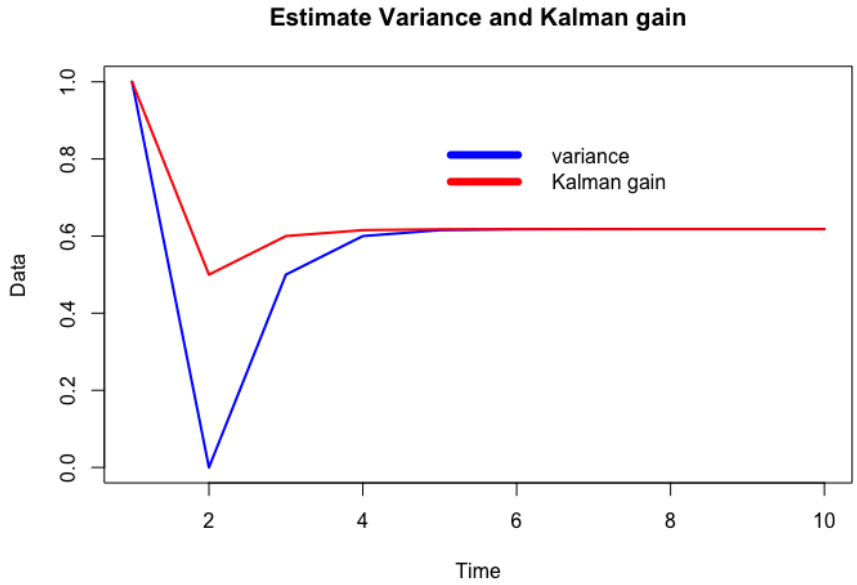
$$k = \frac{\sigma_\eta^2}{\sigma^2 + \sigma_\eta^2}$$

$$\sigma^2(\sigma^2 + \sigma_\eta^2) = \sigma_\epsilon^2 \sigma_\eta^2$$

With the solutions:

$$\sigma^2 = -\frac{\sigma_\eta^2}{2} + \sqrt{\frac{\sigma_\eta^4}{4} + \sigma_\epsilon^2 \sigma_\eta^2}$$

$$k = \frac{\sigma_\eta^2}{\sigma^2 + \sigma_\eta^2}$$




```
> # Initialize the estimate variance and Kalman gain
> nrows <- 10
> vareta <- 1; vareps <- 1
> varv <- numeric(nrows); varv[1] <- 1
> kgain <- numeric(nrows); kgain[1] <- 1
> # Update the variance and Kalman gain
> for (it in 2:nrows) {
+   varv[it] <- (1-kgain[it-1])*(varv[it-1] + vareta)
+   kgain[it] <- (varv[it] + vareta)/(varv[it] + vareta + vareps)
+ }  # end for
> # Plot the variance and Kalman gain
> datav <- cbind(varv, kgain)
> colnames(datav) <- c("variance", "Kalman gain")
> matplot(y=datav, main="Estimate Variance and Kalman gain",
+   xlab="Time", ylab="Data",
+   type="l", lty="solid", lwd=2, col=c("blue", "red"))
> legend(x="topright", legend=colnames(datav),
+  inset=0.1, cex=1.0, bg="white", bty="n", y.intersp=0.4,
+  lwd=6, lty=1, col=c("blue", "red"))
```

The Kalman Gain

The steady state value of the Kalman gain only depends on the ratio of the standard deviation of the observations (measurements) σ_ϵ divided by the standard deviation of the forecasts σ_η.

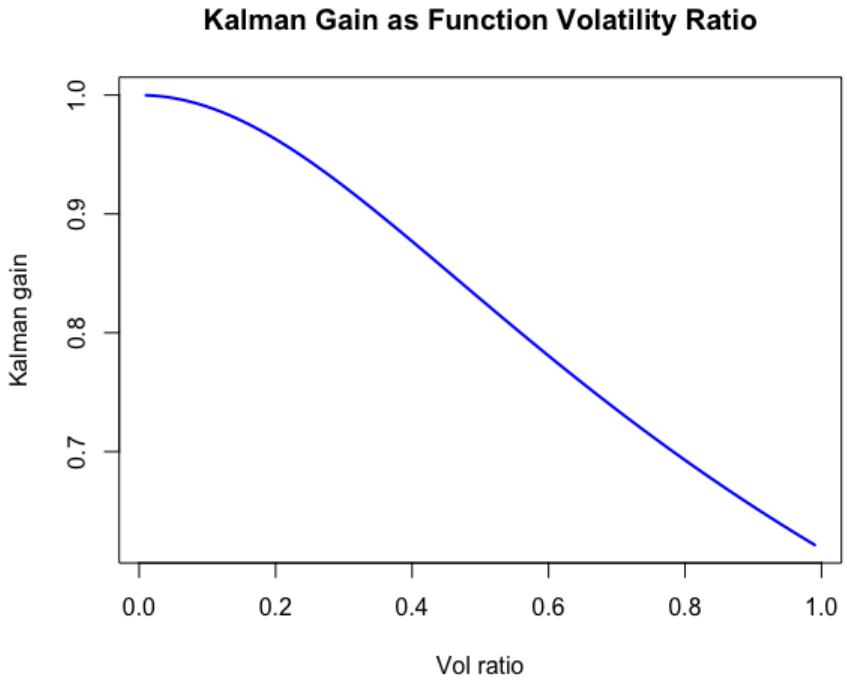
$$\sigma^2 = \sigma_\eta^2(-\frac{1}{2} + \sqrt{\frac{1}{4} + \frac{\sigma_\epsilon^2}{\sigma_\eta^2}})$$

$$k = \frac{1}{\frac{1}{2} + \sqrt{\frac{1}{4} + \frac{\sigma_\epsilon^2}{\sigma_\eta^2}}}$$

For very small observation volatility σ_ϵ, the Kalman gain is close to 1, and the best estimate of the price today $\bar{p}_t$ is the observed value today o_t.

While for very large observation volatility σ_ϵ, the Kalman gain is close to 0, and the best estimate of the price today $\bar{p}_t$ is the estimate from yesterday $\bar{p}_{t-1}$.

$$\bar{p}_t = \bar{p}_{t-1} + k(o_t - \bar{p}_{t-1})$$




```
> # Define Kalman gain function
> kfun <- function(volr) 1/(0.5 + sqrt(0.25 + volr^2))
> # Plot Kalman gain
> curve(expr=kfun, xlim=c(0.01, 0.99),
+   main="Kalman Gain as Function Volatility Ratio",
+   xlab="Vol ratio", ylab="Kalman gain", col="blue", lwd=2)
```

Solution of the Kalman Filter

After the Kalman filter settles into a steady state, the update equation for the price estimate $\bar{p}_t$ becomes:

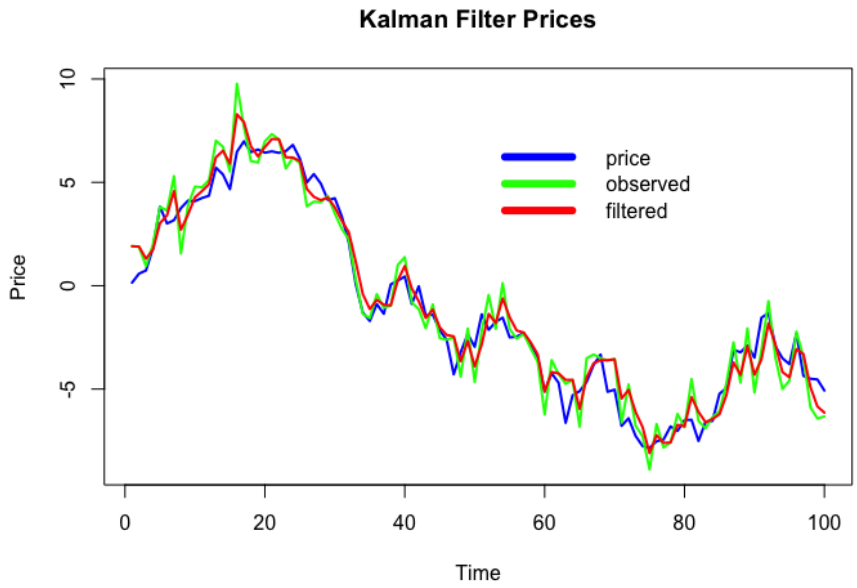
$$\bar{p}_t = \bar{p}_{t-1} + k(o_t - \bar{p}_{t-1})$$

Where o_t is the observed price of p_t.

The previous price estimate $\bar{p}_{t-1}$ is the best forecast for the price today p_t. So the observed price o_t minus the previous price estimate $\bar{p}_{t-1}$ is the forecast error.

So the second term of the update equation can be interpreted as a correction to the best price estimate $\bar{p}_{t-1}$, equal to the forecast error times the Kalman gain.

The Kalman gain determines the strength of the forecast error on the updated price estimate.




```
> # Define Brownian motion prices
> # Initialize the random number generator
> set.seed(1121, "Mersenne-Twister", sample.kind="Rejection")
> nrows <- 100
> pricev <- cumsum(rnorm(nrows))
> # Calculate the observed values
> prico <- pricev + rnorm(nrows)
> # Initialize the price estimates
> priceb <- numeric(nrows)
> priceb[1] <- prico[1]
> # Update the price estimates
> kgain <- (-1+sqrt(5))/2
> for (it in 2:nrows) {
+   priceb[it] <- priceb[it-1] + kgain*(prico[it] - priceb[it-1])
+ }  # end for
```

```
> # Plot the Kalman filter
> pricev <- cbind(pricev, prico, priceb)
> colnames(pricev) <- c("price", "observed", "filtered")
> matplot(y=pricev, main="Kalman Filter Prices",
+   xlab="Time", ylab="Price",
+   type="l", lty="solid", lwd=2, col=c("blue", "green", "red"))
> legend(x="topright", legend=colnames(pricev),
+  inset=0.1, cex=1.0, bg="white", bty="n", y.intersp=0.4,
+  lwd=6, lty=1, col=c("blue", "green", "red"))
```

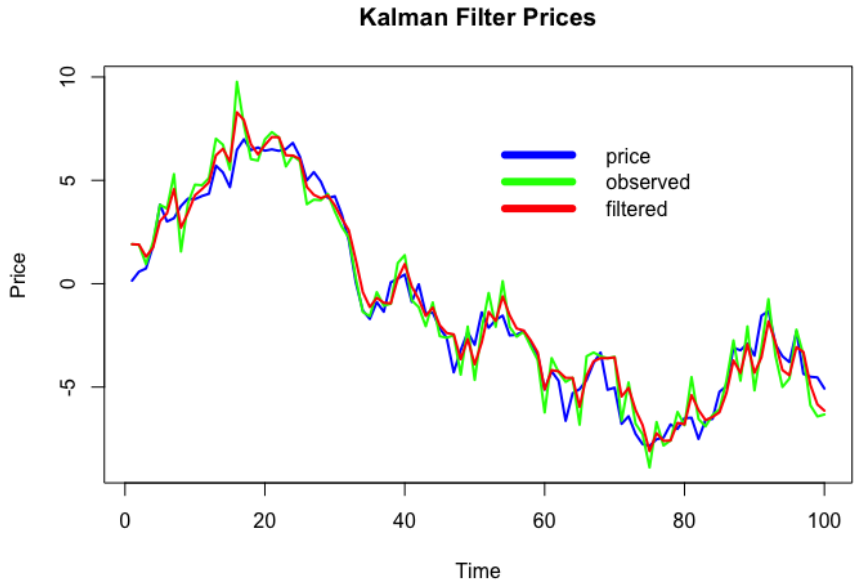
The Kalman Filter and Exponential Smoothing

The update equation can also be written as the *Exponential Moving Average* (*EMA*) of the observed values o_t:

$$\bar{p}_t = (1-k)\bar{p}_{t-1} + ko_t = k\sum_{j=0}^{n}(1-k)^j o_{t-j}$$

The Kalman filtered prices are equal to the *EMA* of the observed values o_t even for more complex processes than Brownian motion, like *ARIMA* processes.

The function `HighFreq::run_mean()` calculates the *EMA* using the `C++` *Armadillo* numerical library.




```
arma::mat run_mean(const arma::mat& tseries,
                   double lambda) {
  arma::uword nrows = tseries.n_rows;
  arma::mat meanm(nrows, tseries.n_cols);
  double lambda1 = 1-lambda;

  meanm.row(0) = tseries.row(0);
  // Calculate the EMA
  for (arma::uword it = 1; it < nrows; it++) {
    // Calculate the means using the decay factor
    meanm.row(it) = lambda*meanm.row(it-1) +
          lambda1*tseries.row(it);
  }  // end for
  return meanm;
}  // end run_mean
```

```
> # Initialize the price estimates
> pricema <- numeric(nrows)
> pricema[1] <- prico[1]
> # Calculate the EMA prices in R
> for (it in 2:nrows) {
+   pricema[it] <- (1-kgain)*pricema[it-1] + kgain*prico[it]
+ }  # end for
> all.equal(pricema, priceb)
> # Calculate the EMA prices using RcppArmadillo C++
> pricpp <- HighFreq::run_mean(matrix(prico), 1-kgain)
> all.equal(drop(pricpp), priceb)
> # Compare the speed of RcppArmadillo C++ with R code
> library(microbenchmark)
> summary(microbenchmark(
+   rcode={for (it in 2:nrows) {
+     pricema[it] <- (1-kgain)*pricema[it-1] + kgain*prico[it]
+   }},
+   cpp=HighFreq::run_mean(matrix(prico), 1-kgain),
```

draft: Classification Using K-Nearest Neighbor (KNN) Algorithm

The K-nearest neighbor (KNN) algorithm is a supervised learning classification technique.

Normalizing numeric data

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

The method `predict.glm()` produces forecasts for a generalized linear model, in the form of probabilities for the `Boolean` response variable.

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

The *null hypothesis* is that `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 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.

draft: Machine Learning Is Not Artificial Intelligence

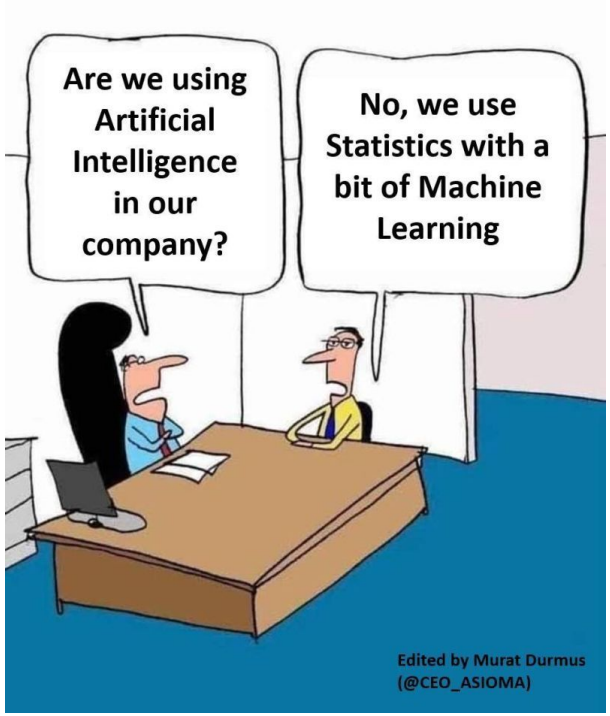
Copy notes from: Systems and Programs.md

Supervised machine Learning a data fitting technique.

The "learning" is merely fitting a function into a set of training data.

The fitted function can then be applied to a test data set to produce predictions.

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



draft: Data Science

Data Science is very important to quantitative finance.

Below is an example of a simulation of the path of *Brownian Motion* crossing a barrier level.

1. Data is never clean.
2. You will spend most of your time cleaning and preparing data.
3. 95% of tasks do not require deep learning.
4. In 90% of cases generalized linear regression will do the trick.
5. Big Data is just a tool.
6. You should embrace the Bayesian approach.
7. No one cares how you did it.
8. Academia and business are two different worlds.
9. Presentation is key – be a master of Power Point.
10. All models are false, but some are useful.
11. There is no fully automated Data Science. You need to get your hands dirty.

draft: Machine Learning

What is Machine Learning? What is Machine Learning? Machine Learning (ML) studies statistical models which can identify patterns in the data and make forecasts. ML is closely related to statistics, but with an emphasis on forecasting. ML models are divided into supervised learning or unsupervised learning. Supervised learning models require a training set to calibrate the model parameters. Examples of supervised learning models are linear regression, decision trees, support vector machines (SVM), and neural networks. Unsupervised learning models don't require a training set. Examples of unsupervised learning models are clustering models, like principal component analysis (PCA) and k-nearest neighbors (KNN). ML models are also divided into classification and regression models. An example of a regression model is linear regression. An example of a classification model is logistic regression. ML uses several techniques to calibrate models and improve forecasting. First, ML uses cross-validation (backtesting) to determine the optimal model meta-parameters. Second, ML uses estimator shrinkage to achieve a better tradeoff between their bias and variance.
Data Science is very important to quantitative finance.

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