FRE6871 R in Finance

Lecture#3, Spring 2026

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Downloading Treasury Bond Rates from *FRED*

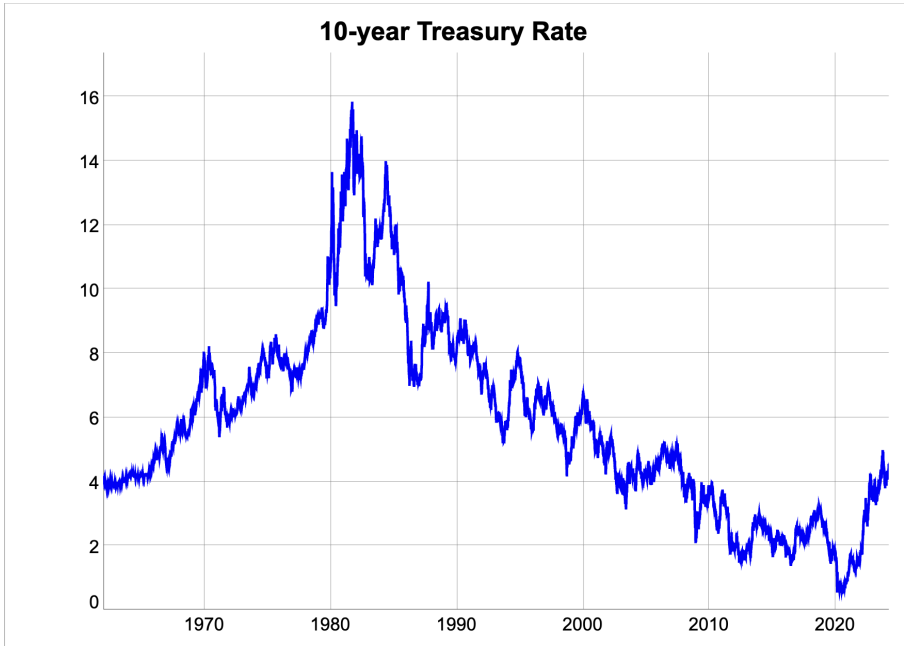
The constant maturity Treasury yields are the yields of hypothetical fixed-maturity bonds, interpolated from the market yields of actual Treasury bonds.

The *FRED* database provides historical constant maturity Treasury yields:

https://fred.stlouisfed.org/series/DGS5

`quantmod::getSymbols()` creates objects in the specified *environment* from the input strings (names).

It then assigns the data to those objects, without returning them as a function value, as a *side effect*.




```
> # Symbols for constant maturity Treasury rates
> symbolv <- c("DGS1", "DGS2", "DGS5", "DGS10", "DGS20", "DGS30")
> # Create new environment for time series
> ratesenv <- new.env()
> # Download time series for symbolv into ratesenv
> quantmod::getSymbols(symbolv, env=ratesenv, src="FRED")
> # Remove NA values in ratesenv
> sapply(ratesenv, function(x) sum(is.na(x)))
> sapply(ls(ratesenv), function(namev) {
+   assign(x=namev, value=na.omit(get(namev, ratesenv)),
+    envir=ratesenv)
+   return(NULL)
+ }) ##  end sapply
> sapply(ratesenv, function(x) sum(is.na(x)))
> # Get class of all objects in ratesenv
> sapply(ratesenv, class)
> # Get class of all objects in R workspace
> sapply(ls(), function(namev) class(get(namev)))
> # Save the time series environment into a binary .RData file
> save(ratesenv, file="/Users/jerzy/Develop/lecture_slides/data/rates_data.RData")
```

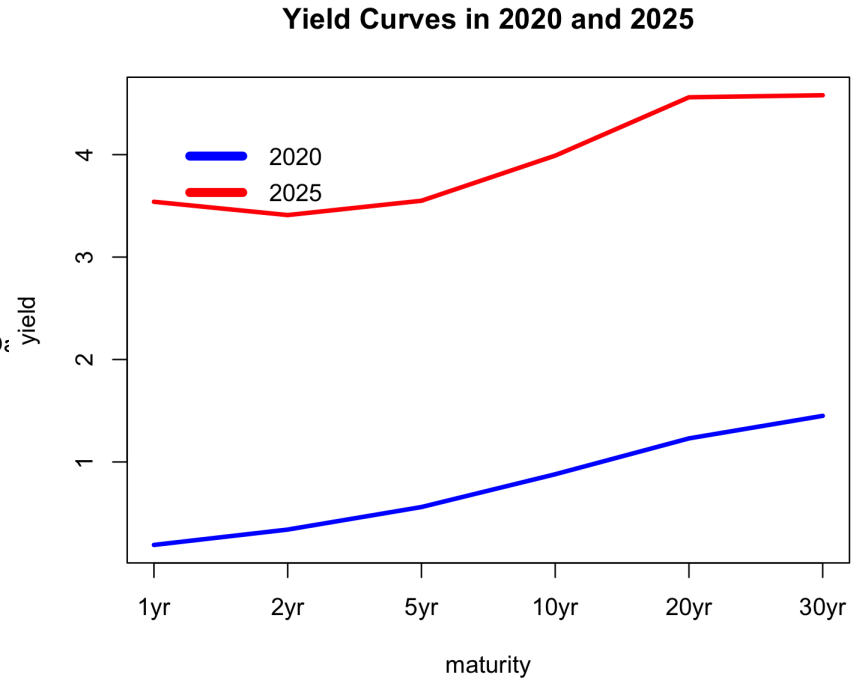
```
> # Get class of time series object DGS10
> class(get(x="DGS10", envir=ratesenv))
> # Another way
> class(ratesenv$DGS10)
> # Get first 6 rows of time series
> head(ratesenv$DGS10)
> # Plot dygraphs of 10-year Treasury rate
> dygraphs::dygraph(ratesenv$DGS10, main="10-year Treasury Rate") %>
+   dyOptions(colors="blue", strokeWidth=2)
> # Plot 10-year constant maturity Treasury rate
> x11(width=6, height=5)
> par(mar=c(2, 2, 0, 0), oma=c(0, 0, 0, 0))
> chart_Series(ratesenv$DGS10["1990/"], name="10-year Treasury Rate"
```

Treasury Yield Curve

The *yield curve* is a vector of interest rates at different maturities, on a given date.

The *yield curve* shape changes depending on the economic conditions: in recessions rates drop and the curve flattens, while in expansions rates rise and the curve steepens.

```
> # Load constant maturity Treasury rates
> load(file="/Users/jerzy/Develop/lecture_slides/data/rates_data.RDa
> # Get most recent yield curve
> ycnow <- eapply(ratesenv, xts::last)
> class(ycnow)
> ycnow <- do.call(cbind, ycnow)
> # Check if 2020-03-25 is not a holiday
> date2020 <- as.Date("2020-03-25")
> weekdays(date2020)
> # Get yield curve from 2020-03-25
> yc2020 <- eapply(ratesenv, function(x) x[date2020])
> yc2020 <- do.call(cbind, yc2020)
> # Combine the yield curves
> ycurves <- c(yc2020, ycnow)
> # Rename columns and rows, sort columns, and transpose into matr
> colnames(ycurves) <- substr(colnames(ycurves), start=4, stop=11)
> ycurves <- ycurves[, order(as.numeric(colnames(ycurves)))]
> colnames(ycurves) <- paste0(colnames(ycurves), "yr")
> ycurves <- t(ycurves)
> colnames(ycurves) <- substr(colnames(ycurves), start=1, stop=4)
```

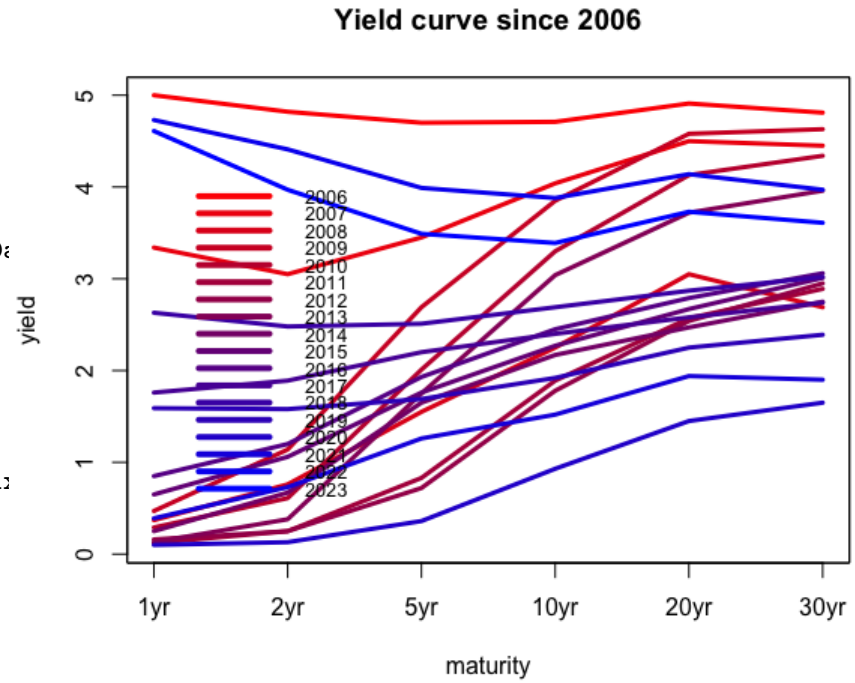



```
> # Plot using matplot()
> colorv <- c("blue", "red")
> matplot(ycurves, main="Yield Curves in 2020 and 2023", xaxt="n",
+   type="l", xlab="maturity", ylab="yield", col=colorv)
> # Add x-axis
> axis(1, seq_along(rownames(ycurves)), rownames(ycurves))
> # Add legend
> legend("topleft", legend=colnames(ycurves), y.intersp=0.5,
+  bty="n", col=colorv, lty=1, lwd=6, inset=0.05, cex=1.0)
```

Treasury Yield Curve Over Time

The *yield curve* changes shape dramatically depending on the economic conditions: in recessions rates drop and the curve flattens, while in expansions rates rise and the curve steepens.

```
> # Load constant maturity Treasury rates
> load(file="/Users/jerzy/Develop/lecture_slides/data/rates_data.RDa
> # Get end-of-year dates since 2006
> datev <- xts::endpoints(ratesenv$DGS1["2006/"], on="years")
> datev <- zoo::index(ratesenv$DGS1["2006/"][datev])
> # Create time series of end-of-year rates
> ycurves <- eapply(ratesenv, function(ratev) ratev[datev])
> ycurves <- rutils::do_call(cbind, ycurves)
> # Rename columns and rows, sort columns, and transpose into matri
> colnames(ycurves) <- substr(colnames(ycurves), start=4, stop=11)
> ycurves <- ycurves[, order(as.numeric(colnames(ycurves)))]
> colnames(ycurves) <- paste0(colnames(ycurves), "yr")
> ycurves <- t(ycurves)
> colnames(ycurves) <- substr(colnames(ycurves), start=1, stop=4)
> # Plot matrix using plot.zoo()
> colorv <- colorRampPalette(c("red", "blue"))(NCOL(ycurves))
> plot.zoo(ycurves, main="Yield Curve Since 2006", lwd=3, xaxt="n"
+    plot.type="single", xlab="maturity", ylab="yield", col=colorv
> # Add x-axis
> axis(1, seq_along(rownames(ycurves)), rownames(ycurves))
> # Add legend
> legend("topleft", legend=colnames(ycurves), y.intersp=0.5,
+  bty="n", col=colorv, lty=1, lwd=4, inset=0.05, cex=0.8)
```




```
> # Alternative plot using matplot()
> matplot(ycurves, main="Yield curve since 2006", xaxt="n", lwd=3,
+   type="l", xlab="maturity", ylab="yield", col=colorv)
> # Add x-axis
> axis(1, seq_along(rownames(ycurves)), rownames(ycurves))
> # Add legend
> legend("topleft", legend=colnames(ycurves), y.intersp=0.5,
+  bty="n", col=colorv, lty=1, lwd=4, inset=0.05, cex=0.8)
```

Nelson-Siegel Yield Curve Model

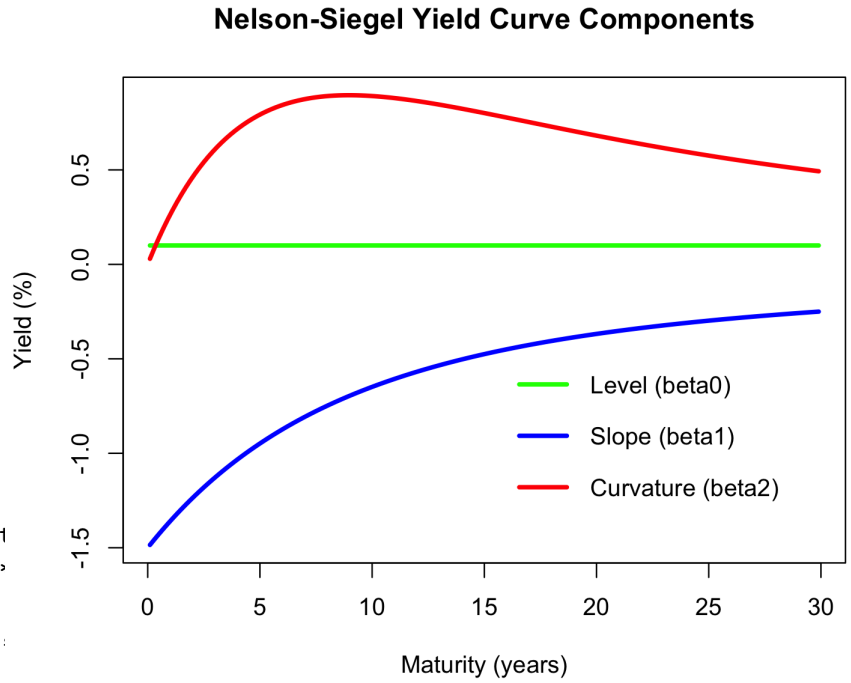
The Nelson-Siegel model of the *yield curve* is given by:

$$y(\tau) = \beta_0 + \beta_1\left(\frac{1 - e^{-\lambda\tau}}{\lambda\tau}\right) + \beta_2\left(\frac{1 - e^{-\lambda\tau}}{\lambda\tau} - e^{-\lambda\tau}\right)$$

Where $y(\tau)$ is the yield at the maturity τ and λ is the time decay factor.

The first term β_0 represents the long-term level of interest rates, the second term β_1 represents the slope, and the third term β_2 represents the curvature of the yield curve.

```
> # Define the Nelson-Siegel model
> slopef <- function(tau, lambda) (1 - exp(-lambda*tau)) / (lambda*t
> curvef <- function(tau, lambda) slopef(tau, lambda) - exp(-lambda*
> nsfun <- function(tau, beta0, beta1, beta2, lambda) {
+   return(beta0 + beta1 * slopef(tau, lambda) + beta2 * curvef(tau,
+ }  ##  end nsfun
```



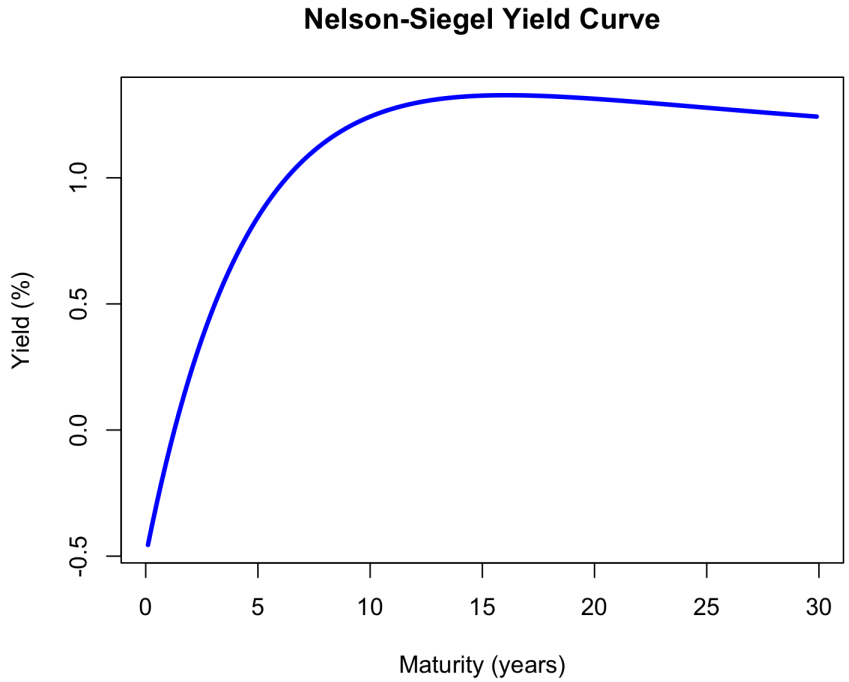

```
> # Plot the Nelson-Siegel components
> tau <- seq(0.1, 30, by=0.2)
> lambda <- 0.2
> beta0 <- 0.1; beta1 <- -1.5; beta2 <- 3.0
> matplot(tau, cbind(beta0, beta1 * slopef(tau, lambda), beta2 * cur
+   type="l", lwd=3, lty=1,
+   col=c("green", "blue", "red"),
+   main="Nelson-Siegel Yield Curve Components",
+   xlab="Maturity (years)", ylab="Yield (%)")
> legend("bottomright", bty="n", col=c("green", "blue", "red"),
+  legend=c("Level (beta0)", "Slope (beta1)", "Curvature (beta2)"),
+  lty=1, lwd=6, inset=0.05, cex=1.0)
```

Nelson-Siegel Yield Curve

For very short maturities ($\tau \to 0$), the Nelson-Siegel yield is equal to $y(0) = \beta_0 + \beta_1 + \beta_2$.

For very long maturities ($\tau \to \infty$), the yield is equal to $y(\infty) = \beta_0$

```
> # Plot the Nelson-Siegel yield curve
> yieldv <- nsfun(tau, beta0, beta1, beta2, lambda)
> plot(tau, yieldv, type="l", lwd=3, col="blue",
+      main="Nelson-Siegel Yield Curve",
+      xlab="Maturity (years)", ylab="Yield (%)")
```

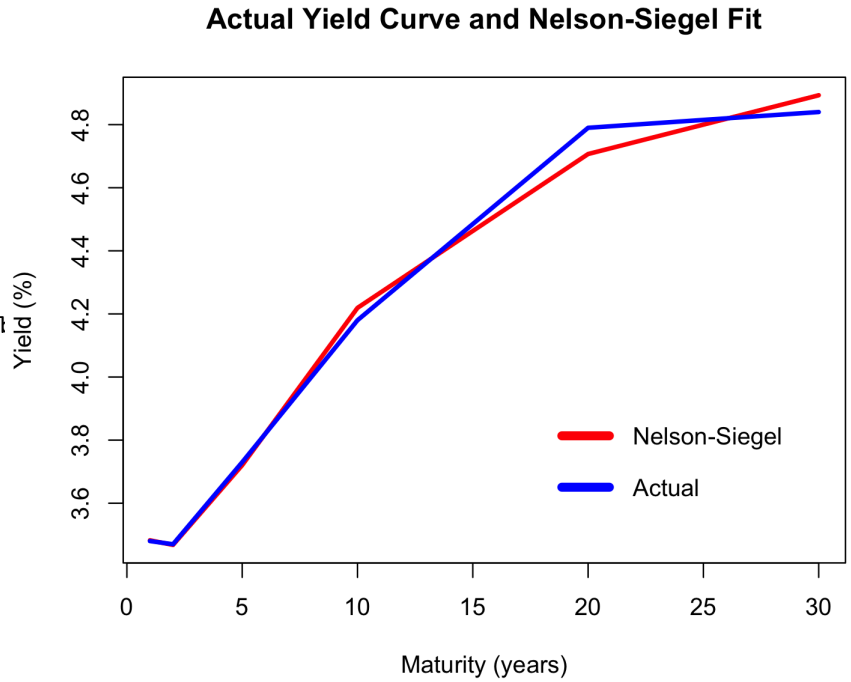



```
> # Plot the Nelson-Siegel yield curve for different values of lambd
> lambdav <- c(0.1, 0.5, 1.0, 2.0)
> yieldm <- sapply(lambdav, function(lambda) {
+   nsfun(tau, beta0, beta1, beta2, lambda)
+ })  ##  end lapply
> matplot(tau, yieldm, type="l", lwd=3, lty=1,
+   col=rainbow(length(lambdav)),
+   main="Nelson-Siegel Yield Curve for Different Lambda",
+   xlab="Maturity (years)", ylab="Yield (%)")
> legend("bottomright", legend=paste0("lambda=", lambdav),
+  bty="n", col=rainbow(length(lambdav)),
+  lty=1, lwd=6, inset=0.05, cex=1.0)
```

Calibrating the Nelson-Siegel Model

The Nelson-Siegel model can be calibrated to the actual yields using the function `optim()`.

```
> # Extract numeric maturities
> yieldv <- ycurves[, "2025"]
> tau <- as.numeric(sub("yr", "", names(yieldv)))
> # Define the Nelson-Siegel model objective function
> objfun <- function(params, tau, yieldv) {
+   beta0 <- params[1]; beta1 <- params[2]; beta2 <- params[3]; lam
+   yieldns <- nsfun(tau, beta0, beta1, beta2, lambda)
+   return(sum((yieldv - yieldns)^2))
+ }  ##  end objfun
> # Calculate objective function value for initial parameters
> objfun(c(beta0, beta1, beta2, lambda), tau=tau, yieldv=yieldv)
> # Optimize parameters using optim()
> pmax <- 30 # Maximum parameter value for optimization
> optim1 <- optim(par=rep(1, 4), # Initial parameter values
+   fn=objfun,
+   tau=tau, yieldv=yieldv,
+   method="L-BFGS-B",
+   upper=rep(pmax, 4),
+   lower=c(-rep(pmax, 3), 0.01))
> # The optimal parameters
> paroptim <- optim1$par
> beta0 <- paroptim[1]; beta1 <- paroptim[2]; beta2 <- paroptim[3]
```



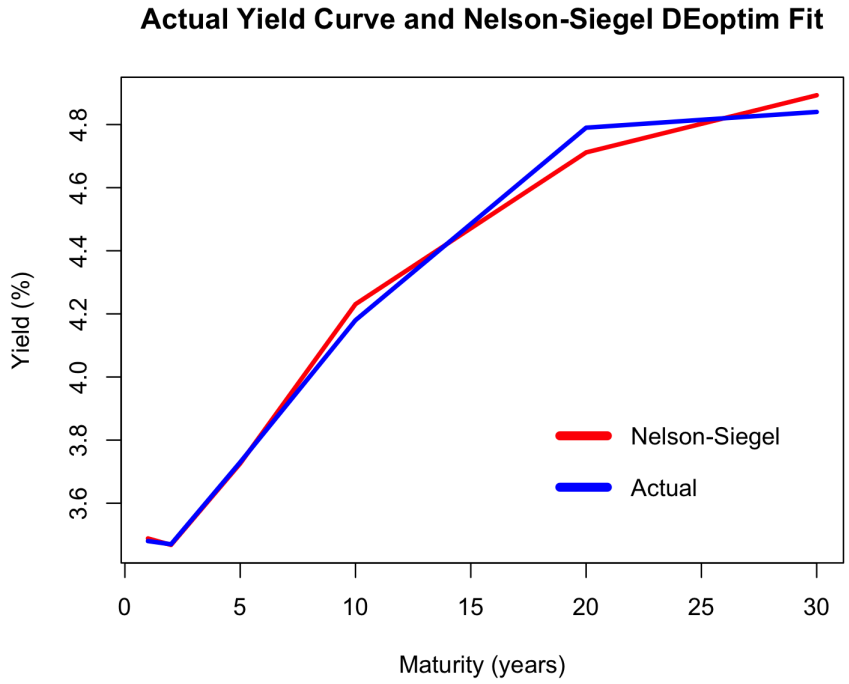

```
> # Plot the Nelson-Siegel yield curve
> yieldv <- nsfun(tau, beta0, beta1, beta2, lambda)
> matplot(tau, cbind(yieldv, ycurves[, "2025"]),
+   type="l", lty=1, lwd=3, col=c("red", "blue"),
+   main="Actual Yield Curve and Nelson-Siegel Fit",
+   xlab="Maturity (years)", ylab="Yield (%)")
> legend("bottomright", legend=c("Nelson-Siegel", "Actual"),
+  bty="n", col=c("red", "blue"),
+  lty=1, lwd=6, inset=0.05, cex=1.0)
```

Calibrating the Nelson-Siegel Model Using Differential Evolution

The Nelson-Siegel model can be calibrated to the actual yields using *global* optimization, to avoid local minima.

The function `DEoptim()` from package *DEoptim* performs *global* optimization using the *Differential Evolution* algorithm.

The function `DEoptim()` is much slower than `optim()`, but it is more likely to find the global minimum of the objective function.




```
> # Extract numeric maturities
> yieldv <- ycurves[, "2025"]
> tau <- as.numeric(sub("yr", "", names(yieldv)))
> # Optimize parameters using DEoptim()
> set.seed(1234)
> library(DEoptim)
> optim1 <- DEoptim::DEoptim(fn = objfun,
+   tau=tau, yieldv=yieldv,
+   upper=rep(pmax, 4),
+   lower=c(-rep(pmax, 3), 0.01),
+   control = DEoptim.control(trace=FALSE, storepopfrom = 1, iterma
> # The optimal parameters
> pardeoptim <- optim1$optim$bestmem
> beta0 <- pardeoptim[1]; beta1 <- pardeoptim[2]; beta2 <- pardeopt
> all.equal(paroptim, pardeoptim, check.attributes=FALSE)
> library(microbenchmark)
> summary(microbenchmark(
+   optim=optim(par=rep(1, 4), fn=objfun, tau=tau, yieldv=yieldv,
+    method="L-BFGS-B", upper=rep(pmax, 4), lower=c(-rep(pmax, 3),
+   deoptim=DEoptim(fn=objfun, tau=tau, yieldv=yieldv,
+    upper=rep(pmax, 4), lower=c(-rep(pmax, 3), 0.01),
+    control=DEoptim.control(trace=FALSE, storepopfrom=1, itermax=500)),
+   times=10))[, c(1, 4, 5)]
```

```
> # Plot the Nelson-Siegel yield curve
> yieldv <- nsfun(tau, beta0, beta1, beta2, lambda)
> matplot(tau, cbind(yieldv, ycurves[, "2025"]),
+   type="l", lty=1, lwd=3, col=c("red", "blue"),
+   main="Actual Yield Curve and Nelson-Siegel DEoptim Fit",
+   xlab="Maturity (years)", ylab="Yield (%)")
> legend("bottomright", legend=c("Nelson-Siegel", "Actual"),
+  bty="n", col=c("red", "blue"),
+  lty=1, lwd=6, inset=0.05, cex=1.0)
```

The Vasicek Interest Rate Model

In the *Vasicek* model is a stochastic process for the short-term interest rate r_t:

$$\mathrm{d}r_t = \theta\left(\mu - r_t\right) + \sigma\,\mathrm{d}B_t$$

Where the parameter σ is the volatility, μ is the equilibrium rate, and θ is the mean reversion parameter.

B_t is a *Brownian Motion*, with its increment $\mathrm{d}B_t$ following the normal distribution with the volatility $\sqrt{\mathrm{d}t}$, equal to the square root of the time increment $\mathrm{d}t$.

The *Vasicek* process is also known as the *Ornstein-Uhlenbeck* process.

The *Vasicek* process is path dependent, so it must be simulated using explicit loops, either in `R` or in `C++`.

The compiled *Rcpp* `C++` code can be over 100 times faster than loops in `R`!

```
> # Define Vasicek parameters
> ratin <- 0.0; rateq <- 4.0;
> sigmav <- 0.1; thetav <- 0.01; nrows <- 1000
> # Initialize the data
> innov <- rnorm(nrows) # innovations
> rated <- numeric(nrows) # rate increments
> ratev <- numeric(nrows) # rates
> rated[1] <- sigmav*innov[1]
> ratev[1] <- ratin
> # Simulate Vasicek process in R
> for (i in 2:nrows) {
+   rated[i] <- thetav*(rateq - ratev[i-1]) + sigmav*innov[i]
+   ratev[i] <- ratev[i-1] + rated[i]
+ }  ##  end for
> # Simulate Vasicek process in Rcpp
> pricecpp <- HighFreq::sim_ou(prici=ratin, priceq=rateq,
+   theta=thetav, innov=matrix(sigmav*innov))
> all.equal(ratev, drop(pricecpp))
> # Compare the speed of R code with Rcpp
> library(microbenchmark)
> summary(microbenchmark(
+   Rcode={for (i in 2:nrows) {
+     rated[i] <- thetav*(rateq - ratev[i-1]) + sigmav*innov[i]
+     ratev[i] <- ratev[i-1] + rated[i]}},
+   Rcpp=HighFreq::sim_ou(prici=ratin, priceq=rateq,
+     theta=thetav, innov=matrix(sigmav*innov)),
+   times=10))[, c(1, 4, 5)]  ##  end microbenchmark summary
```

The Solution of the Vasicek Process

The solution of the *Vasicek* process is given by:

$$r_t = r_0 e^{-\theta t} + \mu(1 - e^{-\theta t}) + \sigma \int_0^t e^{\theta(s-t)} \mathrm{d}B_s$$

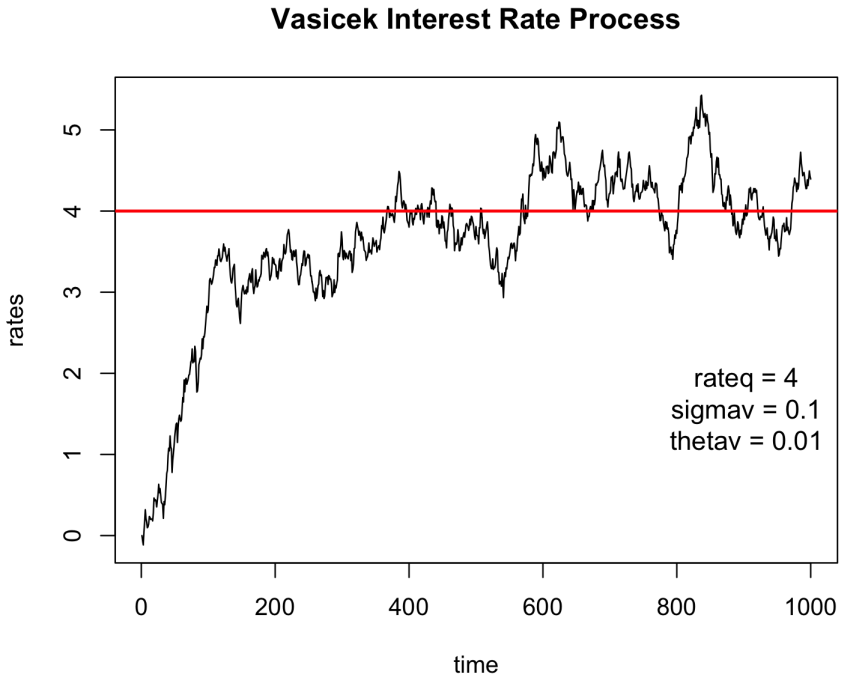
The mean and variance are given by:

$$\mathbb{E}[r_t] = r_0 e^{-\theta t} + \mu(1 - e^{-\theta t}) \to \mu$$

$$\mathbb{E}[(r_t - \mathbb{E}[r_t])^2] = \frac{\sigma^2}{2\theta}(1 - e^{-\theta t}) \to \frac{\sigma^2}{2\theta}$$

The *Vasicek* process is mean reverting to the equilibrium rate μ.

The *Vasicek* process needs a *warmup period* before it reaches equilibrium.

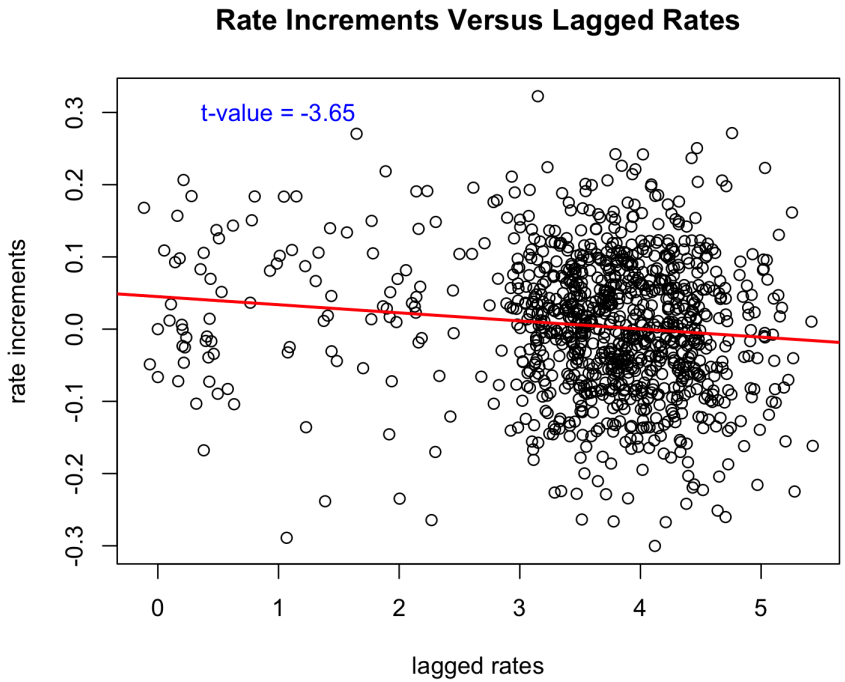



```
> plot(ratev, type="l", xlab="time", ylab="rates",
+      main="Vasicek Interest Rate Process")
> legend("bottomright", title=paste(c(
+   paste0("rateq = ", rateq),
+   paste0("sigmav = ", sigmav),
+   paste0("thetav = ", thetav)),
+   collapse="\n"),
+   legend="", cex=1.1, inset=0.0, bg="white", bty="n")
> abline(h=rateq, col='red', lwd=2)
```

Vasicek Process Increments Correlation

Under the *Vasicek* process, the rate increments are negatively correlated to the lagged rates.

```
> rated <- rutils::diffit(ratev)
> pricelag <- rutils::lagit(ratev)
> formulav <- rated ~ pricelag
> regmod <- lm(formulav)
> summary(regmod)
> # Plot regression
> plot(formulav, xlab="lagged rates", ylab="rate increments",
+      main="Rate Increments Versus Lagged Rates")
> abline(regmod, lwd=2, col="red")
> # Add t-value of the slope
> text(x=1.0, y=0.3, cex=1.0, col="blue",
+  labels=paste("t-value =", round(summary(regmod)$coefficients[2,
```



Calibrating the Vasicek Parameters

The volatility parameter of the Vasicek process can be estimated directly from the standard deviation of the rate increments.

The θ and μ parameters can be estimated from the linear regression of the rate increments versus the lagged prices.

Calculating regression parameters directly from formulas has the advantage of much faster calculations.

```
> # Calculate volatility parameter
> c(volatility=sigmav, estimate=sd(rated))
> # Extract OU parameters from regression
> coeff <- summary(regmod)$coefficients
> # Calculate regression alpha and beta directly
> betac <- cov(rated, pricelag)/var(pricelag)
> alphac <- (mean(rated) - betac*mean(pricelag))
> cbind(direct=c(alpha=alphac, beta=betac), lm=coeff[, 1])
> all.equal(c(alpha=alphac, beta=betac), coeff[, 1],
+     check.attributes=FALSE)
> # Calculate regression standard errors directly
> betac <- c(alpha=alphac, beta=betac)
> fitv <- (alphac + betac*pricelag)
> resids <- (rated - fitv)
> price2 <- sum((pricelag - mean(pricelag))^2)
> betasd <- sqrt(sum(resids^2)/price2/(nrows-2))
> alphasd <- sqrt(sum(resids^2)/(nrows-2)*(1:nrows + mean(pricelag)
> cbind(direct=c(alphasd=alphasd, betasd=betasd), lm=coeff[, 2])
> all.equal(c(alphasd=alphasd, betasd=betasd), coeff[, 2],
+     check.attributes=FALSE)
> # Compare mean reversion parameter theta
> c(theta=(-thetav), round(coeff[2, ], 3))
> # Compare equilibrium rate mu
> c(priceq=rateq, estimate=-coeff[1, 1]/coeff[2, 1])
> # Compare actual and estimated parameters
> coeff <- cbind(c(thetav*rateq, -thetav), coeff[, 1:2])
> rownames(coeff) <- c("drift", "theta")
> colnames(coeff)[1] <- "actual"
> round(coeff, 4)
```

The Yield Curve Under the Vasicek Model

The price of a discount (zero-coupon) bond with maturity T under the *Vasicek* model is given by:

$$P_T = \exp(A_T - B_T\, r_t)$$

Where r_t is the current short rate, and A_T and B_T are functions of the model parameters θ, μ, and σ:

$$B_T = \frac{1 - \exp(-\theta T)}{\theta}$$

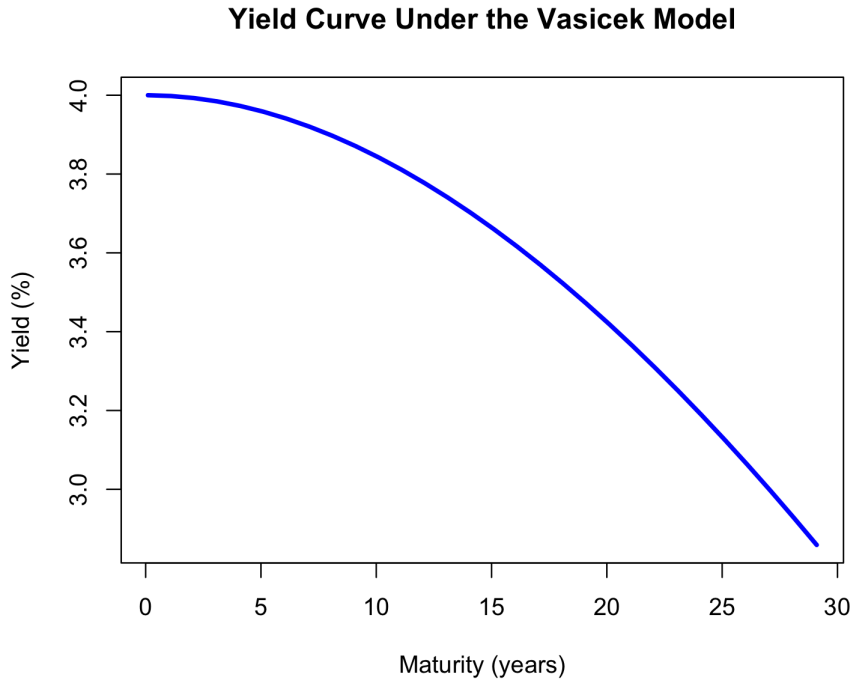
$$A_T = (\mu - \frac{\sigma^2}{2\theta^2})(B_T - T) - \frac{\sigma^2 B_T^2}{4\theta}$$

The discount bond price is $P_T = \exp(-y_T T)$, where the yield to maturity y_T is given by:

$$y_T = \frac{-A_T + B_T\, r_t}{T}$$

The yield curve y_T is a function of the maturity T and the current short rate r_t.

The Vasicek model is a single-factor model because the only source of market risk is the short rate r_t. The level of the short rate r_t determines the whole term structure of interest rates.



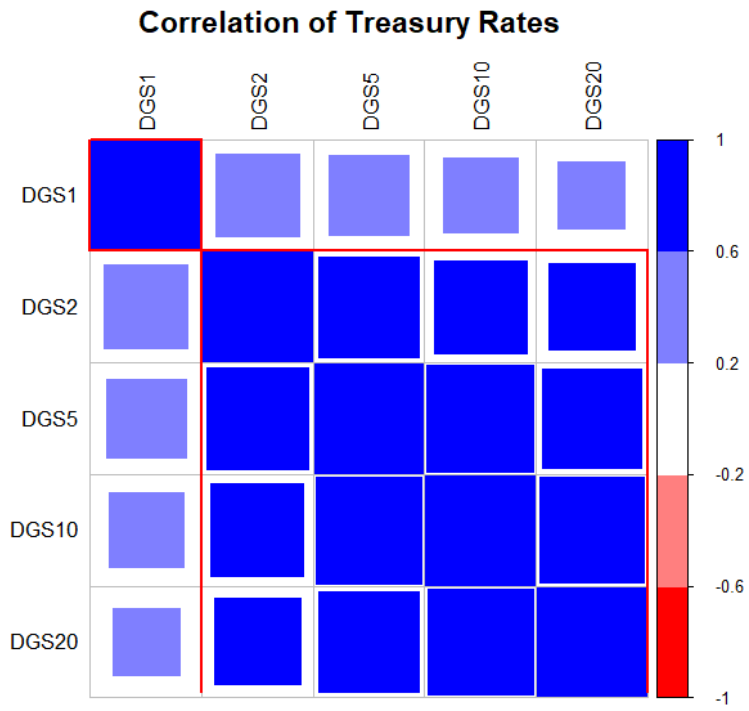

```
> # Calculate the yield curve under the Vasicek model
> Tmax <- 30 # Maximum maturity in years
> Tseq <- seq(0.1, Tmax, by=1.0) # Maturity sequence
> BT <- (1 - exp(-thetav*Tseq))/thetav
> AT <- (rateq - sigmav^2/(2*thetav^2))
> AT <- AT*(BT - Tseq) - (sigmav^2*BT^2)/(4*thetav)
> yieldv <- (-AT + BT*rateq)/Tseq
> # Plot the yield curve
> plot(Tseq, yieldv, type="l", lwd=3, col="blue",
+      main="Yield Curve Under the Vasicek Model",
+      xlab="Maturity (years)", ylab="Yield (%)")
```

Covariance Matrix of Interest Rates

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

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

```
> # Extract rates from ratesenv
> symbolv <- c("DGS1", "DGS2", "DGS5", "DGS10", "DGS20")
> ratem <- mget(symbolv, envir=ratesenv)
> ratem <- rutils::do_call(cbind, ratem)
> ratem <- zoo::na.locf(ratem, na.rm=FALSE)
> ratem <- zoo::na.locf(ratem, fromLast=TRUE)
> # Calculate daily percentage rates changes
> rated <- rutils::diffit(log(ratem))
> # Center (de-mean) the rate increments
> rated <- lapply(rated, function(x) {x - mean(x)})
> rated <- rutils::do_call(cbind, rated)
> sapply(rated, mean)
> # Covariance and Correlation matrices of Treasury rates
> covmat <- cov(rated)
> cormat <- cor(rated)
> # 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"))
> corrplot(cormat, title=NA, tl.col="black",
+     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)
> title("Correlation of Treasury Rates", line=1)
> # Draw rectangles on the correlation matrix plot
> corrRect.hclust(cormat, k=NROW(cormat) %/% 2,
+   method="complete", col="red")
```

Principal Component Vectors

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

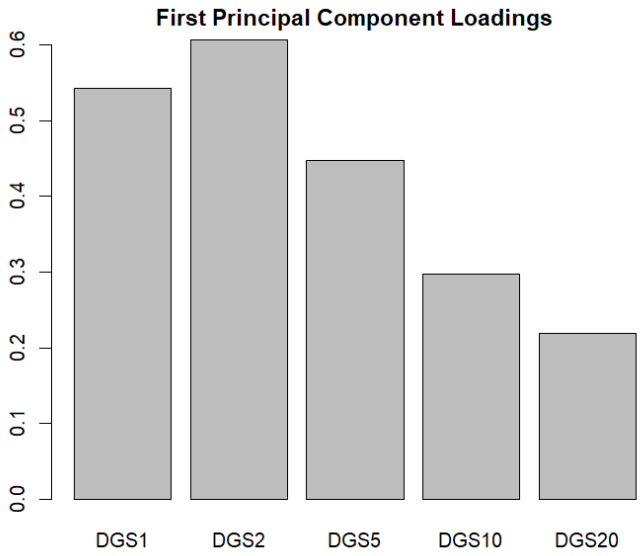
$$\mathbf{pc}_j = \sum_{i=1}^{k} w_{ij}\, \mathbf{r}_i$$

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, rated) {
+   rated <- rated %*% weightv
+   -1e7*var(rated) + 1e7*(1 - sum(weightv*weightv))^2
+ }  ##  end objfun
> # Objective function for equal weight portfolio
> objfun(weightv, rated)
> # Compare speed of vector multiplication methods
> library(microbenchmark)
> summary(microbenchmark(
+   transp=t(rated) %*% rated,
+   sumv=sum(rated*rated),
```

```
> # Find weights with maximum variance
> optim1 <- optim(par=weightv,
+   fn=objfun,
+   rated=rated,
+   method="L-BFGS-B",
+   upper=rep(5.0, nweights),
+   lower=rep(-5.0, nweights))
> # Optimal weights and maximum variance
> weights1 <- optim1$par
> objfun(weights1, rated)
> # Plot first principal component loadings
> x11(width=6, height=5)
> par(mar=c(3, 3, 2, 1), oma=c(0, 0, 0, 0), mgp=c(2, 1, 0))
> barplot(weights1, names.arg=names(weights1),
+   xlab="", ylab="", main="First Principal Component Loadings")
```

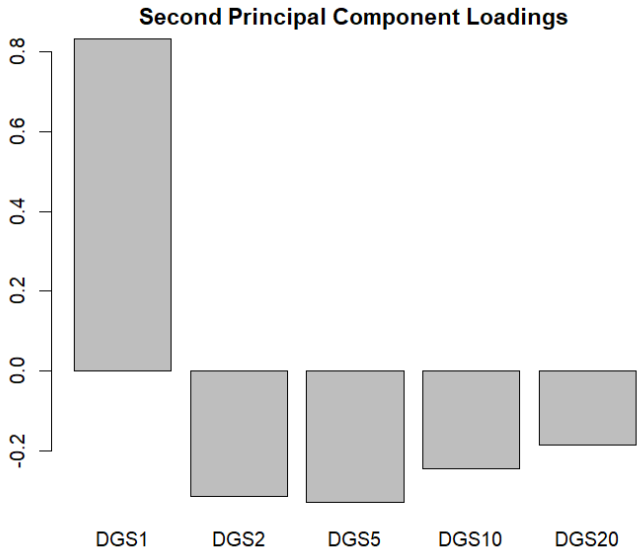
Higher Order Principal Components

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*.

The number of principal components is equal to the dimension of the covariance matrix.

```
> # pc1 weights and rate increments
> pc1 <- drop(rated %*% weights1)
> # Redefine objective function
> objfun <- function(weightv, rated) {
+   rated <- rated %*% weightv
+   -1e7*var(rated) + 1e7*(1 - sum(weightv^2))^2 +
+     1e7*sum(weights1*weightv)^2
+ }  ##  end objfun
> # Find second principal component weights
> optiml <- optim(par=weightv,
+              fn=objfun,
+              rated=rated,
+              method="L-BFGS-B",
+              upper=rep(5.0, nweights),
+              lower=rep(-5.0, nweights))
```




```
> # pc2 weights and rate increments
> weights2 <- optiml$par
> pc2 <- drop(rated %*% weights2)
> sum(pc1*pc2)
> # Plot second principal component loadings
> barplot(weights2, names.arg=names(weights2),
+   xlab="", ylab="", main="Second Principal Component Loadings")
```

Eigenvalues of the Covariance 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* $\mathcal{L}$:

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

Where λ is a *Lagrange multiplier*.

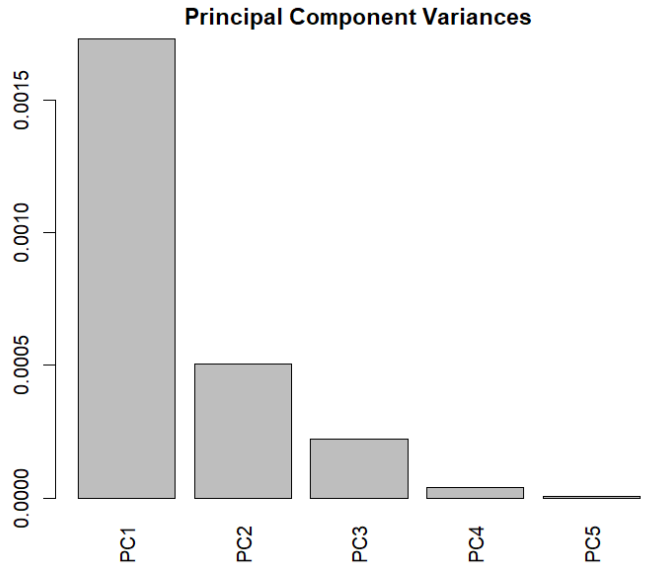
The maximum variance portfolio weights can be found by differentiating $\mathcal{L}$ with respect to $\mathbf{w}$ and setting it to zero:

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

The above 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:

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




```
> eigend <- eigen(covmat)
> eigend$vectors
> # Compare with optimization
> all.equal(sum(diag(covmat)), sum(eigend$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 are satisfied approximately
> (covmat %*% weights1) / weights1 / var(pc1)
> (covmat %*% 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 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.

```
> # Eigen decomposition of correlation matrix
> eigend <- eigen(cormat)
> # Perform PCA with scaling
> pcad <- prcomp(rated, 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(rated, scale=FALSE)
> # Compare outputs
> all.equal(eigend$values, pcad$sdev^2)
> all.equal(abs(eigend$vectors), abs(pcad$rotation),
+     check.attributes=FALSE)
```

Principal Component Analysis of the Yield Curve

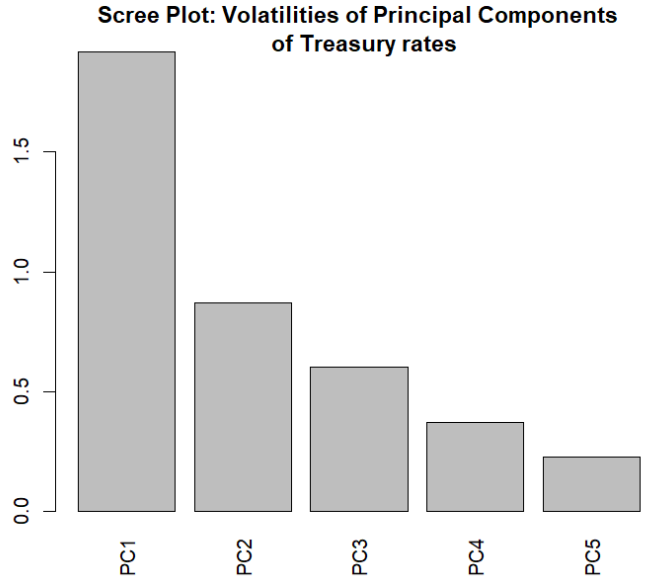
Principal Component Analysis (*PCA*) can be used for *dimension reduction*, to explain a large number of correlated time series as linear combinations of a smaller number of principal component time series.

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.



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

```
> # Perform principal component analysis PCA
> pcad <- prcomp(rated, scale=TRUE)
> # Plot standard deviations
> barplot(pcad$sdev, names.arg=colnames(pcad$rotation),
+   las=3, xlab="", ylab="",
+   main="Scree Plot: Volatilities of Principal Components
+   of Treasury rates")
```

Yield Curve Principal Component Loadings (Weights)

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

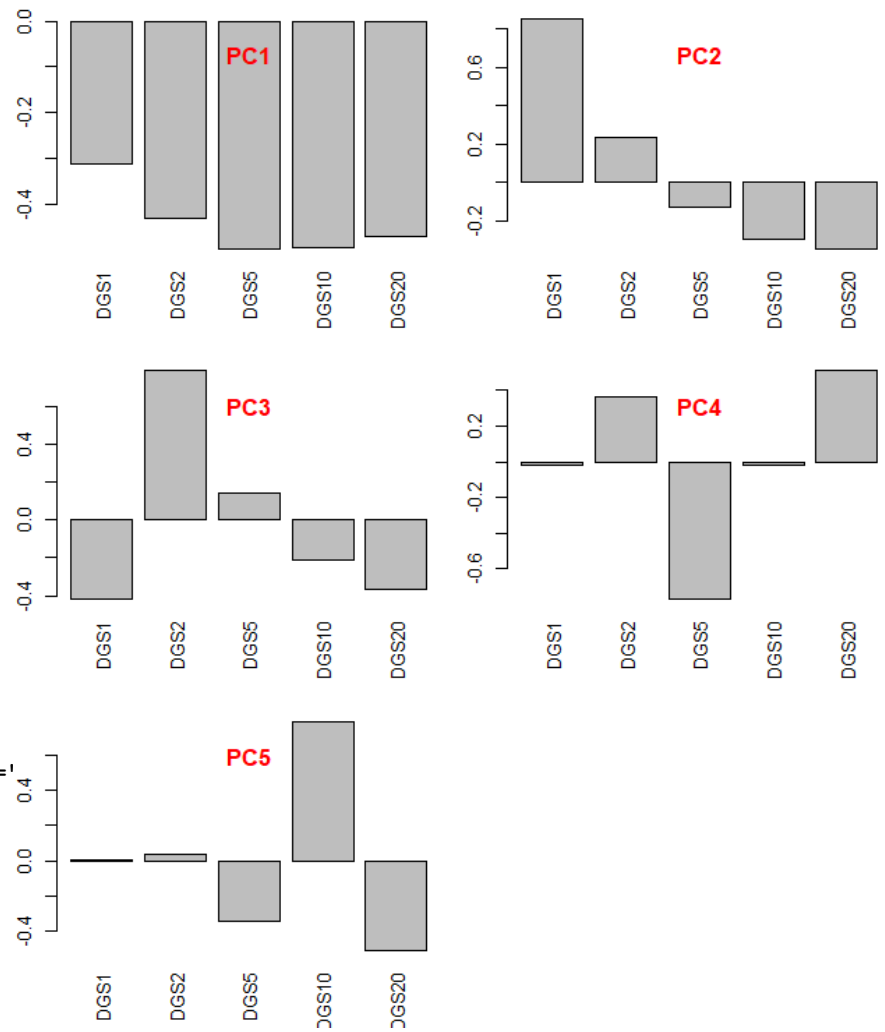
The *principal component* portfolios represent the different orthogonal modes of the data variance.

The first *principal component* of the *yield curve* is the correlated movement of all rates up and down.

The second *principal component* is *yield curve* steepening and flattening.

The third *principal component* is the *yield curve* butterfly movement.

```
> # Calculate principal component loadings (weights)
> pcad$rotation
> # Plot loading barplots in multiple panels
> par(mfrow=c(3,2))
> par(mar=c(3.5, 2, 2, 1), oma=c(0, 0, 0, 0))
> for (ordern in 1:NCOL(pcad$rotation)) {
+   barplot(pcad$rotation[, ordern], las=3, xlab="", ylab="", main='
+   title(paste0("PC", ordern), line=-2.0, col.main="red")
+ }  ##  end for
```



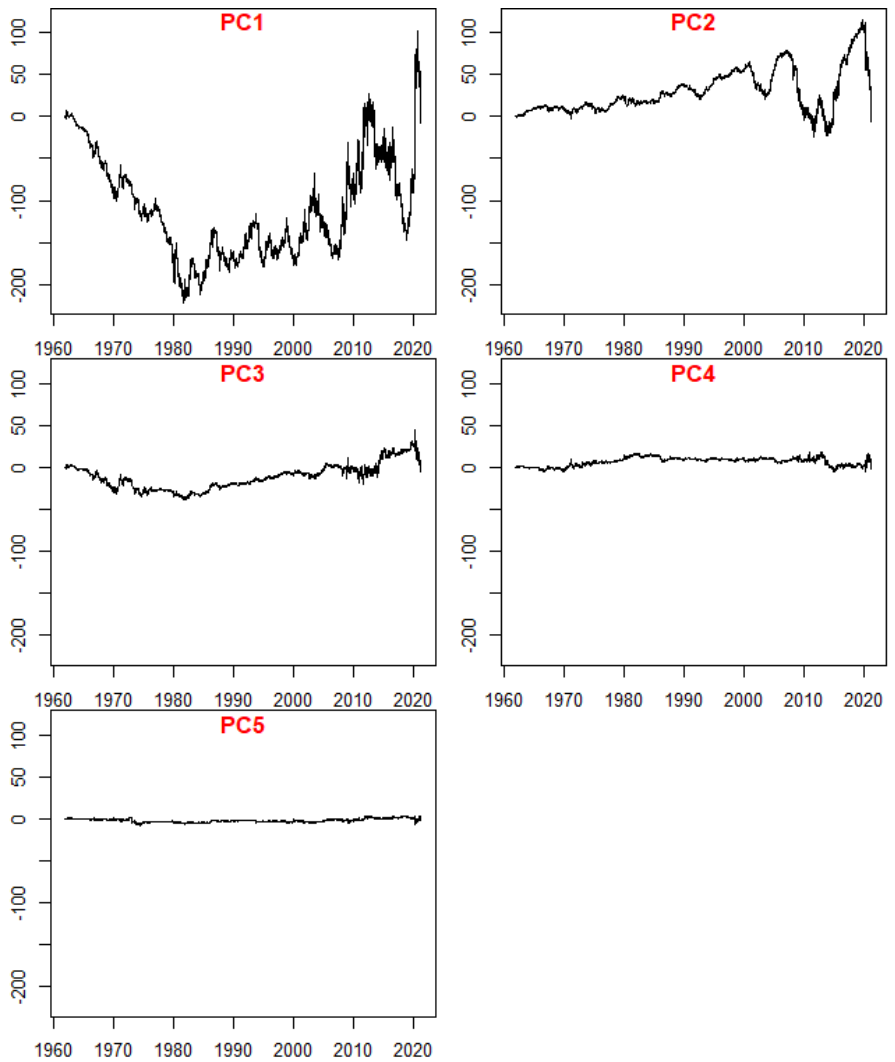
Yield Curve Principal Component Time Series

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 rate increments.

Higher order *principal components* are gradually less volatile.

```
> # Standardize (center and scale) the rate increments
> rated <- lapply(rated, function(x) {(x - mean(x))/sd(x)})
> rated <- rutils::do_call(cbind, rated)
> sapply(rated, mean)
> sapply(rated, sd)
> # Calculate principal component time series
> ratepca <- rated %*% pcad$rotation
> all.equal(pcad$x, ratepca, check.attributes=FALSE)
> # Calculate products of principal component time series
> round(t(ratepca) %*% ratepca, 2)
> # Coerce to xts time series
> ratepca <- xts(ratepca, order.by=zoo::index(rated))
> ratepca <- cumsum(ratepca)
> # Plot principal component time series in multiple panels
> par(mfrow=c(3,2))
> par(mar=c(2, 2, 0, 1), oma=c(0, 0, 0, 0))
> rangev <- range(ratepca)
> for (ordern in 1:NCOL(ratepca)) {
+   plot.zoo(ratepca[, ordern], ylim=rangev, xlab="", ylab="")
+   title(paste0("PC", ordern), line=-1, col.main="red")
+ }  ##  end for
```



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

```
> # Invert all the principal component time series
> ratepca <- rated %*% pcad$rotation
> solved <- ratepca %*% solve(pcad$rotation)
> all.equal(coredata(rated), solved)
```

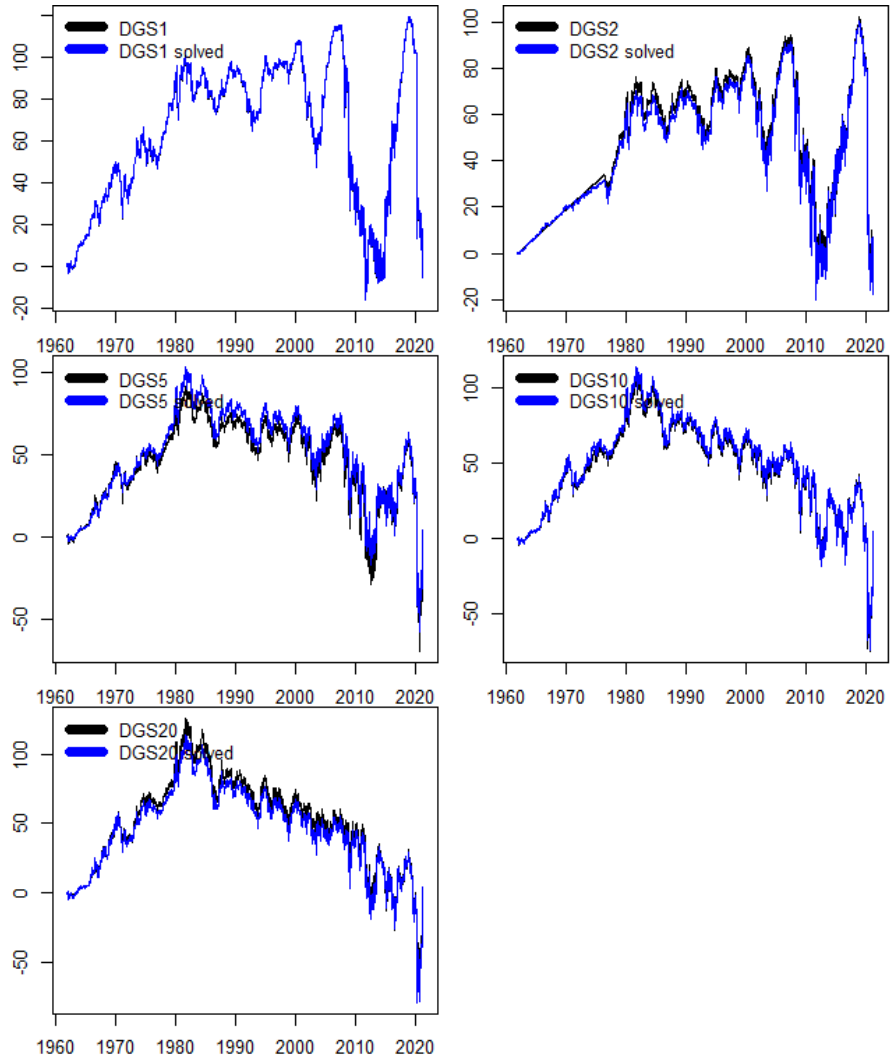
Dimension Reduction Using Principal Component Analysis

The original time series can be calculated *approximately* from just the first few *principal components*, which demonstrates how *PCA* can be used for *dimension reduction*.

A popular rule of thumb is to use the *principal components* with the largest variances, which sum up to 80% of the total variance of rate increments.

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

```
> # Invert first 3 principal component time series
> solved <- ratepca[, 1:3] %*% solve(pcad$rotation)[1:3, ]
> solved <- xts::xts(solved, zoo::index(rated))
> solved <- cumsum(solved)
> retc <- cumsum(rated)
> # Plot the solved rate increments
> par(mfrow=c(3,2))
> par(mar=c(2, 2, 0, 1), oma=c(0, 0, 0, 0))
> 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", y.intersp=0.5,
+    legend=paste0(symboln, c("", " solved")),
+    title=NULL, inset=0.0, cex=1.0, lwd=6,
+    lty=1, col=c("black", "blue"))
+ }  ##  end for
```



Conservation of Variance in PCA

The matrix of *principal component* rate increments **pc** is equal to the matrix **w** of the PCA weights (loadings) times the matrix of the return vectors **r**:

$$\mathbf{pc} = \mathbf{w}\,\mathbf{r}$$

Where the PCA weights $\mathbf{w}^T\mathbf{w} = \mathbb{1}$ are orthonormal.

So the sum of the PCA variances is equal to:

$$\mathbf{pc}^T\mathbf{pc} = (\mathbf{w}\,\mathbf{r})^T\mathbf{w}\,\mathbf{r} = \mathbf{r}^T\,(\mathbf{w}^T\mathbf{w})\,\mathbf{r} = \mathbf{r}^T\mathbf{r}$$

So the total variance is conserved in PCA: the sum of the PCA variances is equal to the sum of the factor variances.

```
> # Calculate the PC time series
> pcad <- prcomp(rated, scale=FALSE)
> ratepca <- rated %*% pcad$rotation
> # Compare the total variances
> all.equal(sum(apply(ratepca, 2, var)), sum(apply(rated, 2, var)))
```

Calibrating Yield Curve Using Package *RQuantLib*

The package *RQuantLib* is an interface to the *QuantLib* open source C/C++ library for quantitative finance, mostly designed for pricing fixed-income instruments and options.

The function `DiscountCurve()` calibrates a *zero coupon yield curve* from *money market* rates, *Eurodollar* futures, and *swap* rates.

The function `DiscountCurve()` interpolates the *zero coupon* rates into a vector of dates specified by the `times` argument.

```
> library(RQuantLib)  ##  Load RQuantLib
> # Specify curve parameters
> curvep <- list(tradeDate=as.Date("2018-01-17"),
+          settleDate=as.Date("2018-01-19"),
+          dt=0.25,
+          interpWhat="discount",
+          interpHow="loglinear")
> # Specify market data: prices of FI instruments
> pricev <- list(d3m=0.0363,
+          fut1=96.2875,
+          fut2=96.7875,
+          fut3=96.9875,
+          fut4=96.6875,
+          s5y=0.0443,
+          s10y=0.05165,
+          s15y=0.055175)
> # Specify dates for calculating the zero rates
> datev <- seq(0, 10, 0.25)
> # Specify the evaluation (as of) date
> setEvaluationDate(as.Date("2018-01-17"))
> # Calculate the zero rates
> ratev <- DiscountCurve(params=curvep, tsQuotes=pricev, times=datev
> # Plot the zero rates
> x11()
> plot(x=ratev$zerorates, t="l", main="zerorates")
```

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.

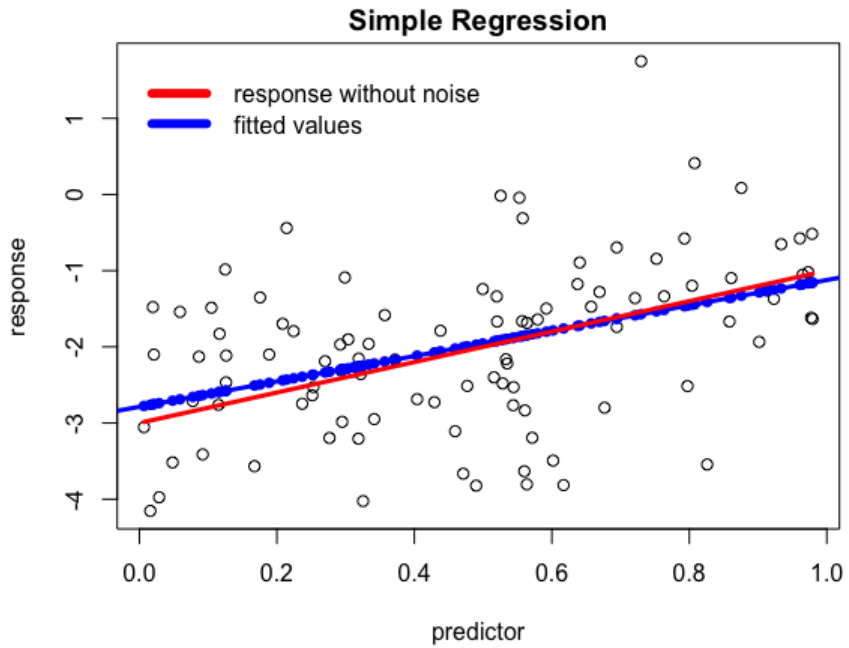
In the Ordinary Least Squares method (*OLS*), the regression parameters are estimated by minimizing the *Residual Sum of Squares* (*RSS*):

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

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

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

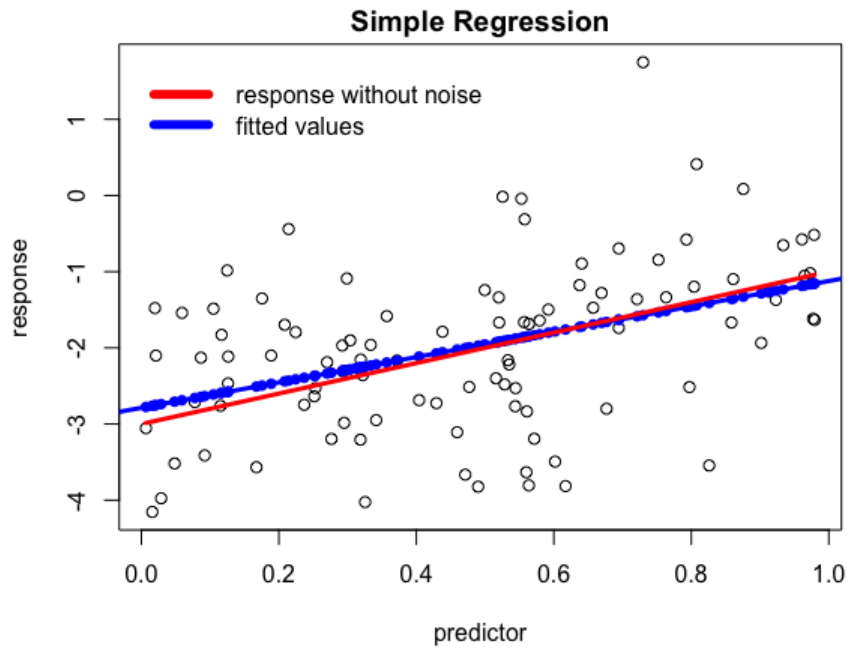
The *fitted values* y_{fit} are the estimates of the *response vector* obtained from the regression model:

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

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")
```



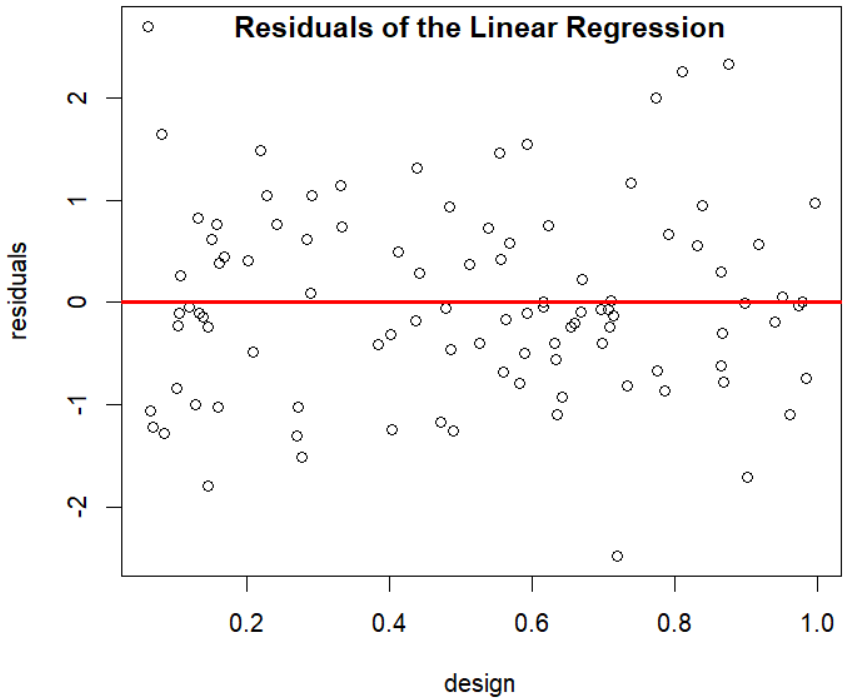

```
> # Plot response without noise
> lines(x=predm, y=(respv-noisev), col="red", lwd=3)
> legend(x="topleft", ##  Add legend
+        legend=c("response without noise", "fitted values"),
+        title=NULL, inset=0.0, cex=1.0, y.intersp=0.3,
+        bty="n", lwd=6, lty=1, col=c("red", "blue"))
```

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)
> residv <- (respv - fitv)
> all.equal(residv, regmod$residuals, check.attributes=FALSE)
[1] TRUE
> # Residuals are orthogonal to the predictor
> all.equal(sum(residv*predm), target=0)
[1] TRUE
> # Residuals are orthogonal to the fitted values
> all.equal(sum(residv*fitv), target=0)
[1] TRUE
> # Sum of residuals is equal to zero
> all.equal(mean(residv), 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* ε_i can be considered the source of error and uncertainty in the *response vector* y:
$y_i = \alpha + \beta x_i + \varepsilon_i$.

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:

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

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

```
> # 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
> residvd <- sqrt(sum(residv^2)/degf)
> # Standard error of beta
> betasd <- residvd/sqrt(sum(predc^2))
> # Standard error of alpha
> alphasd <- residvd*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
```

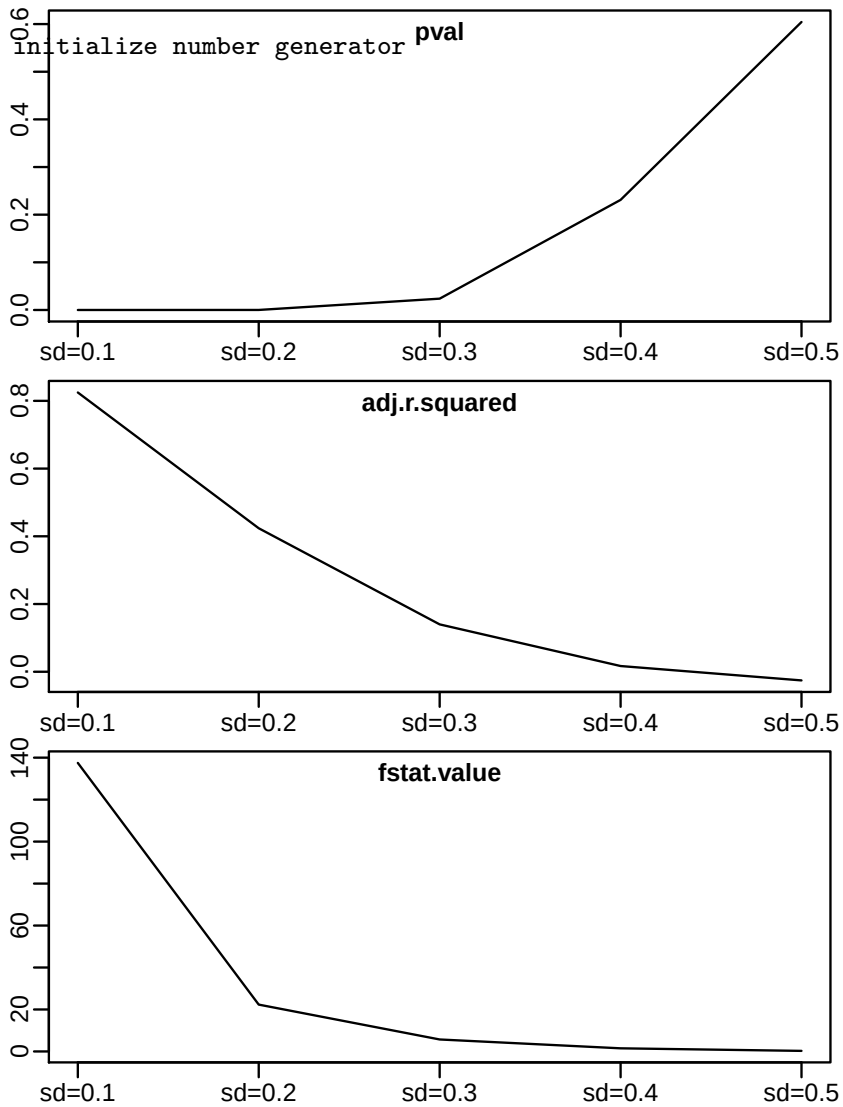
Weak Regression

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
```

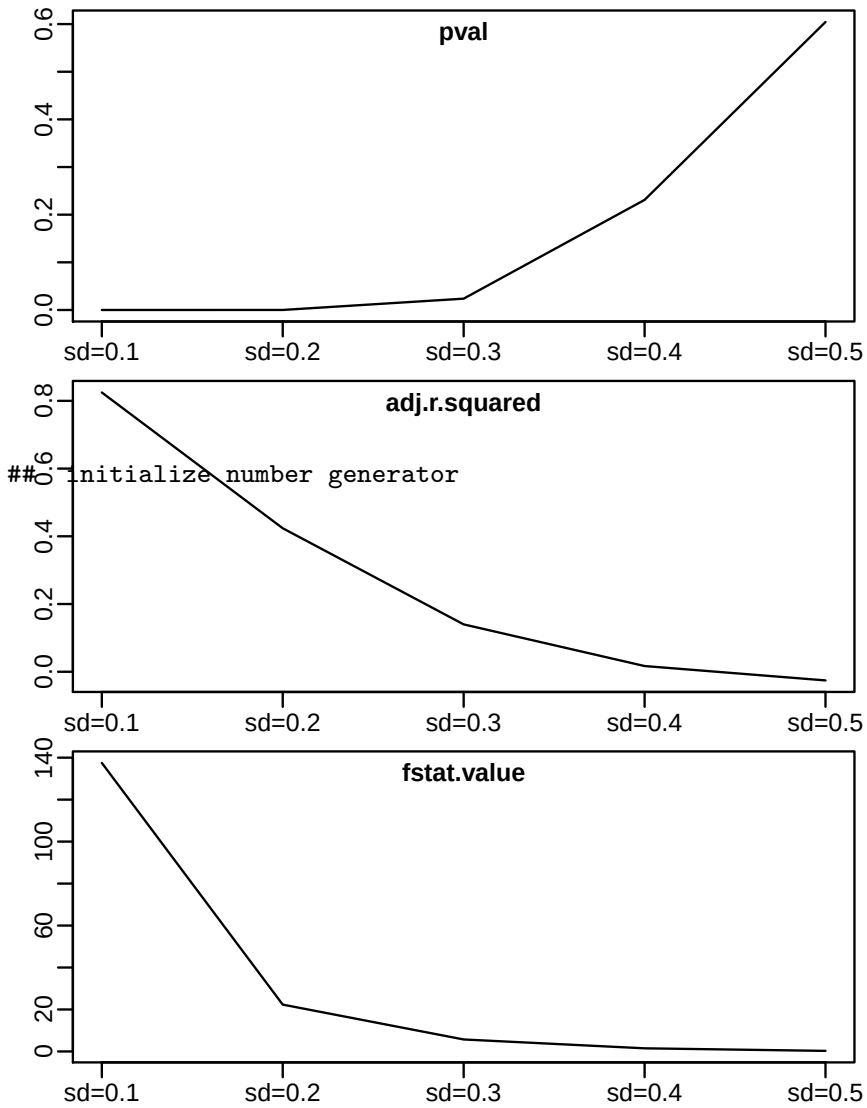
Influence of Noise on Regression

```
> 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
+   colv <- colnames(datav)
+   formulav <- paste(colv[2], colv[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")
+ # 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
```



initialize number generator

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.

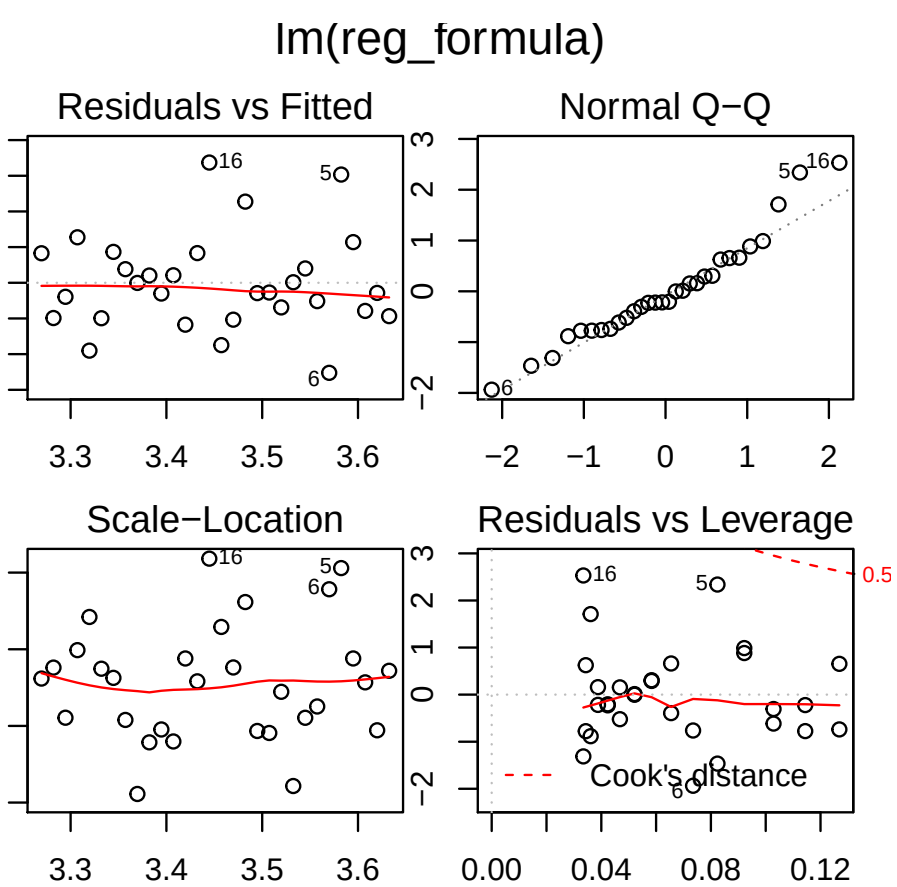
"Residuals vs Leverage" is a scatterplot of the residuals vs. their leverage.

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
```

Univariate Regression in Homogeneous Form

The *linear regression* can be written in *homogeneous form* by defining a *predictor matrix* $\mathbb{X} = (\mathbb{1}, x)$ with two columns, with the unit column representing the intercept:

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

The two *regression coefficients* are combined into a vector: $\beta = (\alpha, \beta)$.

The solution for the regression coefficients β is given by:

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

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

The generalized inverse $\mathbb{X}^{-1}$ satisfies the equation:

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

Which is a generalization of the inverse property: $\mathbb{X}^{-1}\mathbb{X} = \mathbb{1}$.

```
> # Define predictor matrix
> set.seed(1121, "Mersenne-Twister", sample.kind="Rejection")
> nrows <- 100
> predm <- runif(nrows)
> # Define response with noise
> noisev <- rnorm(nrows)
> respv <- (-3 + 2*predm + noisev)
> # Solve the regression using lm()
> formulav <- respv ~ predm
> regmod <- lm(formulav)  ##  Perform regression
> betalm <- regmod$coeff  ##  Regression coefficients
> # Add unit column to predictor
> predm <- cbind(rep(1, nrows), predm)
> colnames(predm)[1] <- "intercept"
> # Calculate the generalized inverse
> predinv <- MASS::ginv(predm)
> # Generalized inverse property is satisfied
> all.equal(predm %*% predinv %*% predm, predm)
[1] TRUE
> # Solve the regression using the generalized inverse
> betac <- drop(predinv %*% respv)
> all.equal(betalm, betac, check.attributes=FALSE)
[1] TRUE
```

The *Influence Matrix* of Univariate Regression

The fitted values y_{fit} are equal to the response y multiplied by the *influence matrix* H:

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

Where $\mathbb{H} = \mathbb{X}(\mathbb{X}^T\mathbb{X})^{-1}\mathbb{X}^T$ is the *influence matrix*.

The *influence matrix* projects the response vector y onto the regression line, to obtain the fitted values y_{fit}.

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

For univariate regression, 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 is due to the influence of the regression intercept α, and the second term is due to the influence of the regression slope β.

```
> # Calculate the influence matrix
> infmat <- predm %*% predinv
> # The influence matrix is idempotent
> all.equal(infmat, infmat %*% infmat)
> # Calculate the fitted values using influence matrix
> fitv <- drop(infmat %*% respv)
> all.equal(fitv, regmod$fitted.values, check.attributes=FALSE)
> # Calculate the fitted values from regression coefficients
> fitv <- drop(predm %*% betac)
> all.equal(fitv, regmod$fitted.values, check.attributes=FALSE)
```

Covariance Matrix of Fitted Values in Univariate Regression

The response values y can be considered to be *random variables* $\hat{y}$. Then the fitted values y_{fit} are also *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:

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

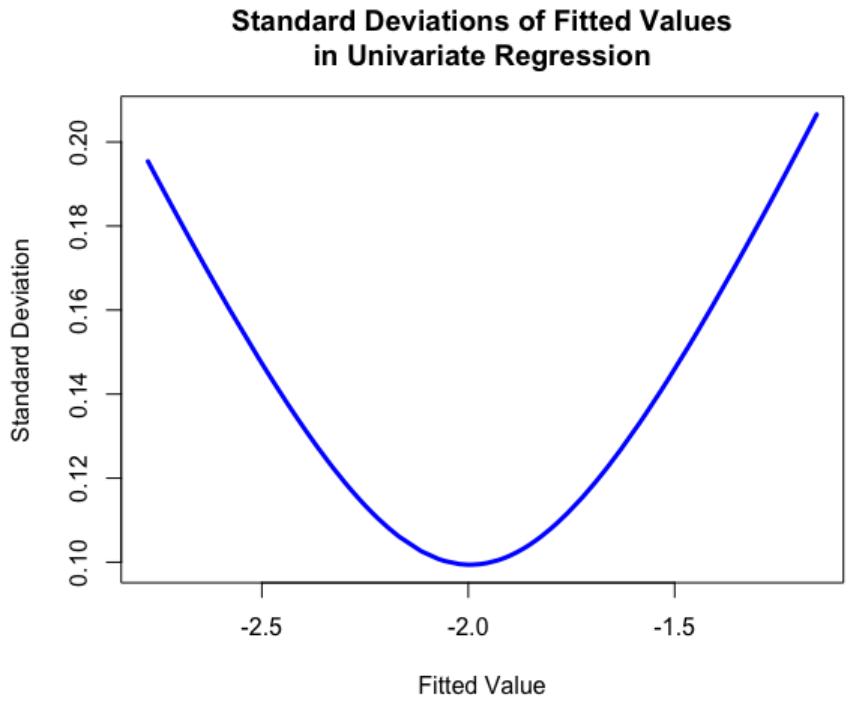
The variance of the fitted values σ^2_{fit} increases with the distance of the *predictors* from their mean values.

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

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

The leverage is the amount by which the fitted values would change if the response values were shifted by a small amount.

The response values farther away from their mean have more *leverage*, that is, more influence on the fitted values, than response values close to the mean.




```
> # Calculate the covariance and standard deviations of fitted value
> residv <- drop(respv - fitv)
> degf <- (NROW(predm) - NCOL(predm))
> residvd <- sqrt(sum(residv^2)/degf)
> fitcovar <- residvd*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
```

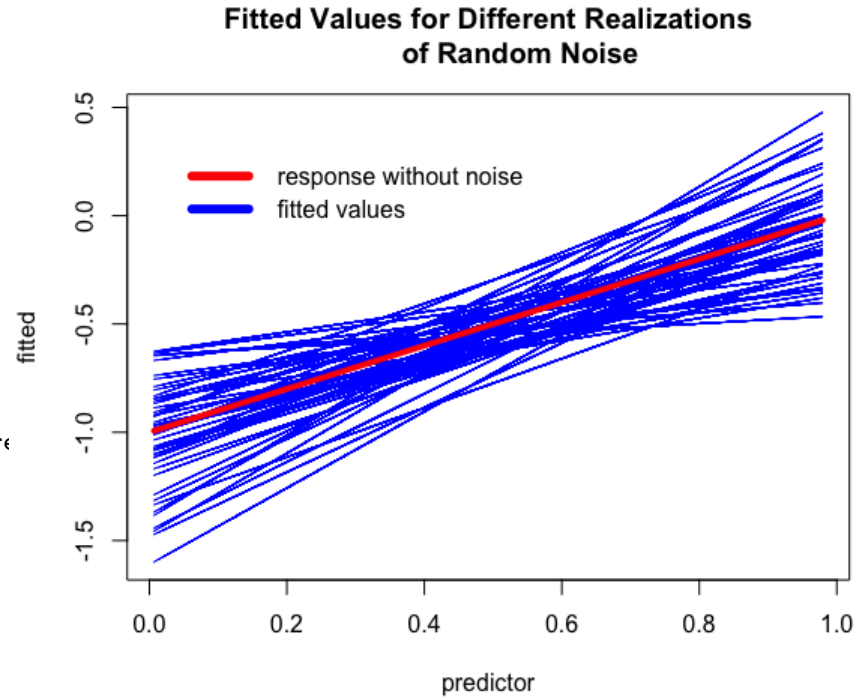
Fitted Values for Different Realizations of Random Noise

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:

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

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

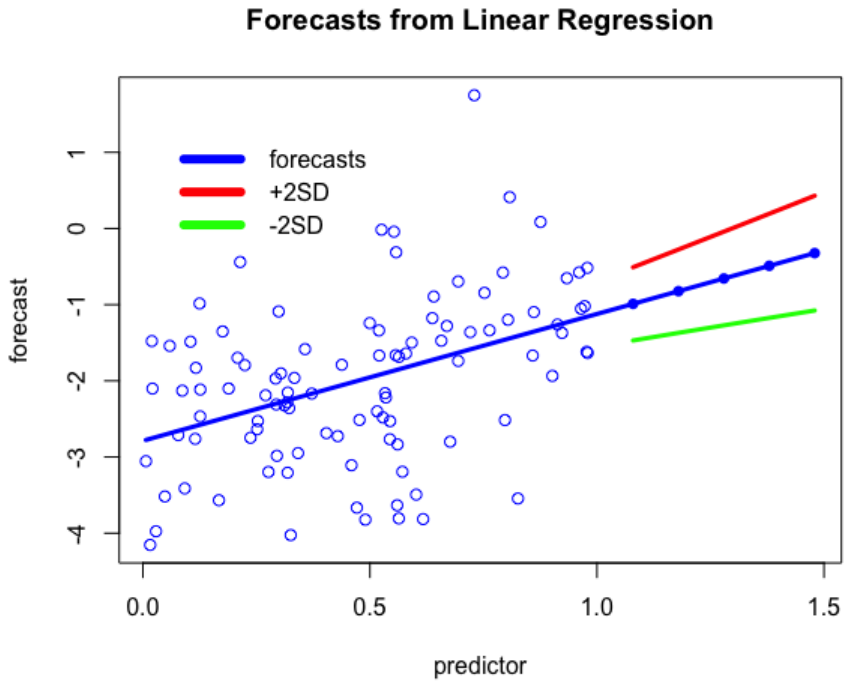
$$\sigma_\varepsilon^2\,\mathbb{X}_{new}(\mathbb{X}^T\mathbb{X})^{-1}\mathbb{X}_{new}^T = \mathbb{X}_{new}\,\sigma_\beta^2\,\mathbb{X}_{new}^T$$

```
> # 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 squared predictor matrix
> pred2 <- MASS::ginv(crossprod(predm))
> # Calculate the standard errors
> predsd <- residvd*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"))
```

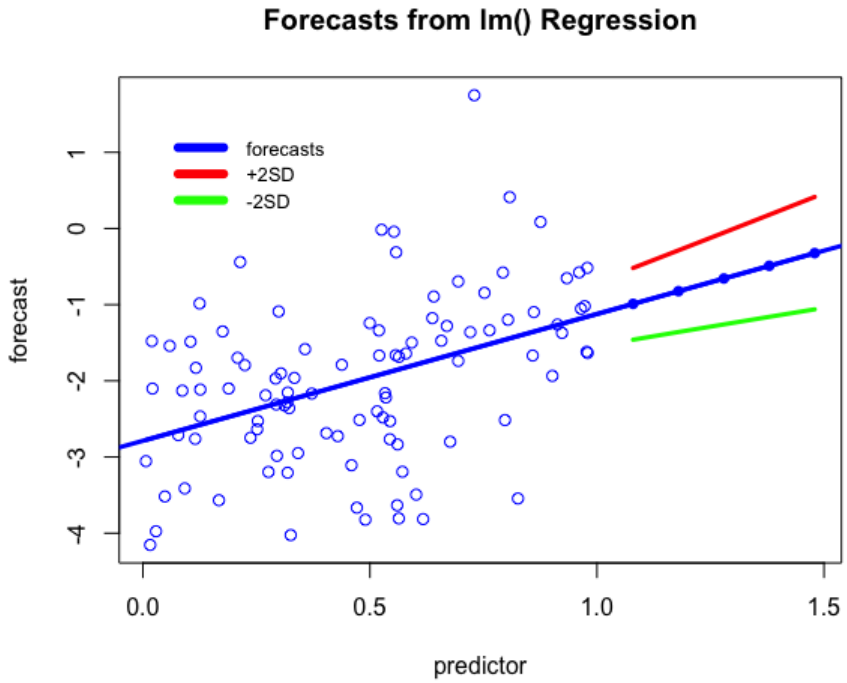


Forecasts of *Linear Regression* Using `predict.lm()`

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

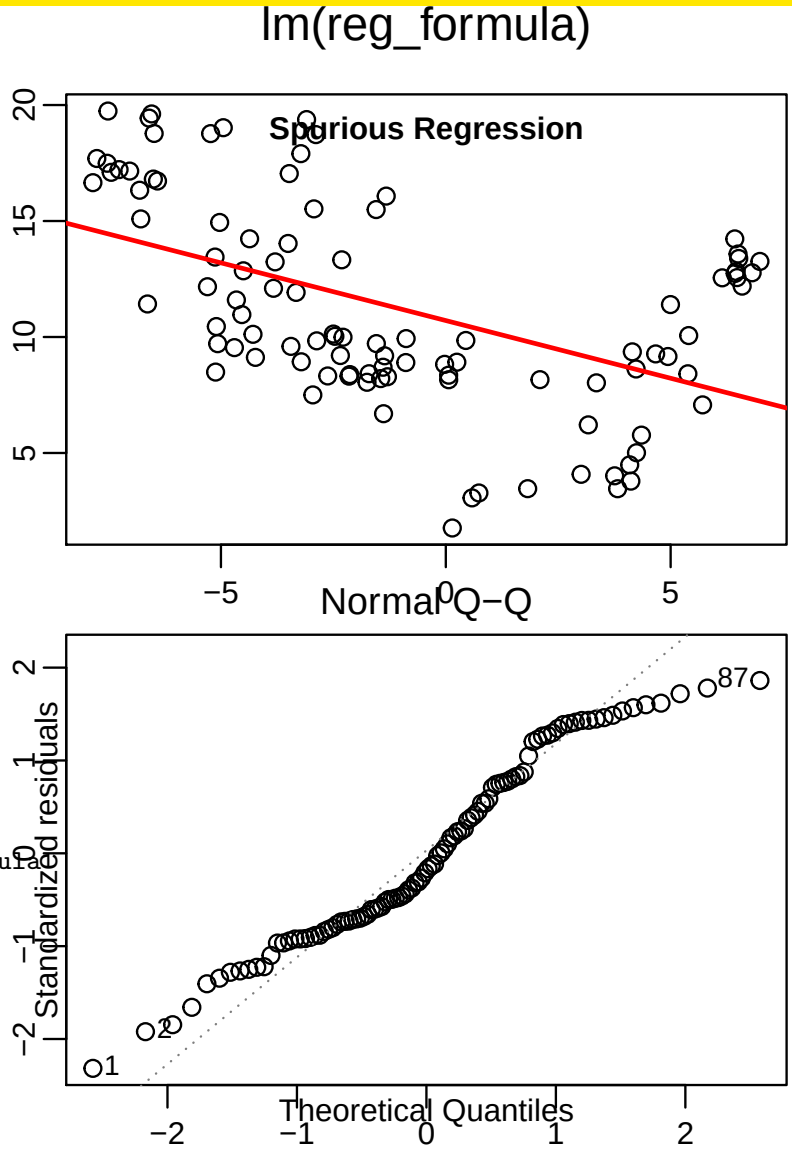
Regression of non-stationary time series creates *spurious* regressions.

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 formulae
> 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

If an extra unit column is added to the *predictor matrix* $\mathbb{X} = (\mathbb{1}, \mathbb{X})$ for the intercept term, then the *linear regression* can be written 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$fitted.values, check.attributes=FALSE)
[1] TRUE
> # Calculate the residuals
> residv <- drop(respv - fitv)
> all.equal(residv, regmod$residuals, check.attributes=FALSE)
[1] TRUE
> # Residuals are orthogonal to predictor columns (predms)
> sapply(residv %*% predm, all.equal, target=0)
[1] TRUE TRUE TRUE TRUE TRUE TRUE
> # Residuals are orthogonal to the fitted values
> all.equal(sum(residv*fitv), target=0)
[1] TRUE
> # Sum of residuals is equal to zero
> all.equal(sum(residv), target=0)
[1] TRUE
```

Solution of Regression Using Coordinate Descent

Multivariate regression can also be solved recursively using *coordinate descent*:

$$r_j = y - \sum_{i \neq j} \beta_i x_i = y - \mathbb{X}_{-j} \beta_{-j}$$

$$\beta_j = \frac{x_j r_j}{x_j^T x_j}$$

The *partial residual* r_j is first calculated without the effect of the j-th *predictor*.

Then the updated *coefficient* β_j is equal to the projection of the *partial residual* r_j onto the j-th *predictor* vector x_j divided by the sum of squared *predictor* vector x_j.

The calculation is repeated until the *regression coefficients* β converge.

```
> # Solve multivariate regression using coordinate descent
> solve_cd <- function(respv, predm, maxit = 1000, tol = 1e-6) {
+   # Initialize the variables
+   ncols <- NCOL(predm)
+   colsq <- colSums(predm^2)
+   betav <- rep(0, ncols)
+   # Loop over iterations
+   for (iter in 1:maxit) {
+     betap <- betav
+     # Loop over the predictors
+     for (j in 1:ncols) {
+       # Calculate the partial residual excluding current predictor
+       residv <- respv - predm[, -j] %*% betav[-j]
+       # Calculate the product of predictor j with the residual
+       covp <- sum(predm[, j] * residv)
+       # Update beta_j coefficient
+       betav[j] <- covp / colsq[j]
+     } # end for j
+     # Break when converged
+     if (sum(abs(betav - betap)) < tol) break
+   } # end for iter
+   return(betav)
+ } # end solve_cd
> # Calculate the regression coefficients using coordinate descent
> betav <- solve_cd(respv, predm)
> all.equal(betav, drop(betac), check.attributes=FALSE)
[1] "Mean relative difference: 6.12e-07"
```

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$fitted.values - mean(respv),
+   check.attributes=FALSE)
[1] TRUE
> # Calculate the residuals
> respc <- respv - mean(respv)
> residv <- drop(respc - fittedc)
> all.equal(residv, regmod$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
> # Calculate the variance of residuals
> residvd <- sum(residv^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* $\mathbb{X}$.

```
> # Calculate the fitted values and the residuals
> fitv <- drop(predm %*% betav)
> residv <- drop(respv - fitv)
> # Calculate the variance of residuals
> degf <- (NROW(predm) - NCOL(predm))
> residvd <- sum(residv^2)/degf
> # Calculate the covariance matrix of betas
> covm <- residvd*pred2

Error:  object 'pred2' not found

> # round(covm, 3)
> betasd <- sqrt(diag(covm))

Error:  object 'covm' not found

> all.equal(betasd, regsum$coeff[, 2], check.attributes=FALSE)
[1] "Numeric: lengths (1, 6) differ"
> # Calculate the t-values of betas
> betatvals <- drop(betac)/betasd
> all.equal(betatvals, regsum$coeff[, 3], check.attributes=FALSE)
[1] "Mean relative difference: 0.492"
> # 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] "Mean relative difference: 1.87"
> # 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:

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

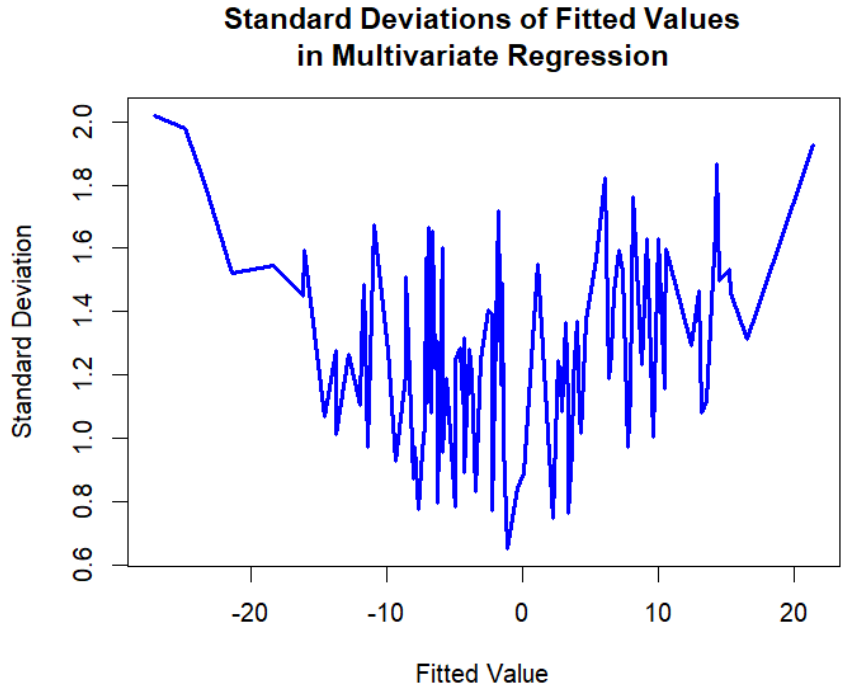
$$\frac{\mathbb{H}\,\mathbb{E}[\hat{\varepsilon}\hat{\varepsilon}^T]\,\mathbb{H}^T}{d_{free}} = \sigma^2_{\varepsilon}\,\mathbb{H} = \sigma^2_{\varepsilon}\,\mathbb{X}(\mathbb{X}^T\mathbb{X})^{-1}\mathbb{X}^T$$

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 <- residvd*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 stock returns shows that the actual standard errors can be much larger as the theoretical standard errors reported by the function `lm()`.

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

```
> # Load time series of ETF percentage returns
> retp <- rutils::etfenv$returns[, c("XLF", "XLE")]
> retp <- na.omit(retp)
> nrows <- NROW(retp)
> head(retp)
> # Define regression formula
> formulav <- paste(colnames(retp)[1],
+   paste(colnames(retp)[-1], collapse="+"),
+   sep=" ~ ")
> # Standard regression
> regmod <- lm(formulav, data=retp)
> regsum <- summary(regmod)
> cdata <- coredata(retp)
> plot(cdata[, 1], cdata[, 2],
+   xlab="XLE", ylab="XLF", main="Stock Returns")
> abline(regmod, lwd=3, col="red")
> # Bootstrap of regression
> set.seed(1121, "Mersenne-Twister", sample.kind="Rejection")
> bootd <- sapply(1:100, function(x) {
+   samplev <- sample.int(nrows, replace=TRUE)
+   regmod <- lm(formulav, data=retp[samplev, ])
+   regmod$coefficients
+ })  ##  end sapply
> # Means and standard errors from regression
> regsum$coefficients
> # Means and standard errors from bootstrap
> 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))
> colv <- colnames(predm)
> colnames(newdata) <- colv
> newdata <- as.matrix(newdata)
> fcast <- drop(newdata %*% betac)
> predsd <- drop(sqrt(newdata %*% covm %*% t(newdata)))

Error:  object 'covm' not found
```

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=regmod, 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*), the *Explained Sum of Squares* (*ESS*), and the *Residual Sum of Squares* (*RSS*) 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 $(y_{fit} - \bar{y})$:

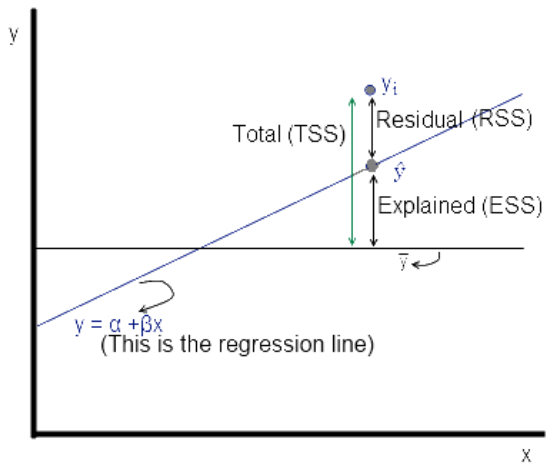
$$(y - y_{fit})^T (y_{fit} - \bar{y}) = 0$$

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(residv^2)
> all.equal(tss, ess + rss)
[1] "Mean relative difference: 7.37e-08"
```

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:

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

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

The *R-squared* measures how well the fitted values fit the response values, but it doesn't measure the statistical significance of the regression.

A regression may have a large *R-squared*, but the coefficient *p*-values may also be large, when the statistical significance of the regression is low.

```
> # 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] "Mean relative difference: 4.85e-07"
> # Correlation between response and fitted values
> corfit <- drop(cor(respv, fitv))
> # Squared correlation between response and fitted values
> all.equal(corfit^2, rsquared)
[1] "Mean relative difference: 4.85e-07"
```

Adjusted R-squared of Multivariate Regression

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

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

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

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

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

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

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

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

Fisher's *F-distribution*

Fisher's *F-distribution* is the distribution of the ratio of two independent sample variances, i.e. two independent *Chi-squared* random variables divided by their respective degrees of freedom.

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:

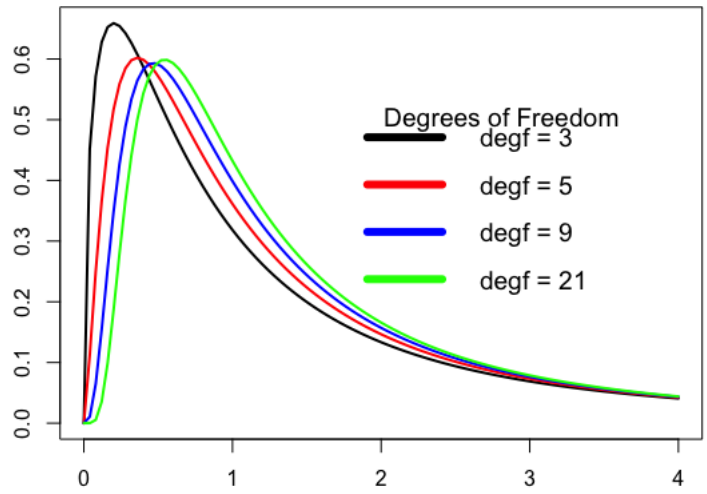
$$F = \frac{\chi^2_m / m}{\chi^2_n / n}$$

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 $m-1$ and $n-1$ degrees of freedom.

The *null hypothesis* of the *F-test* test is that the *F-statistic* 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* 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* 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* data.

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 their *Residual Sum of Squares* RSS_1 and RSS_2 are independent *chi-squared* random variables with df_1 and df_2 degrees of freedom.

And their difference $(RSS_1 - RSS_2)$ follows a *chi-squared* distribution with $(df_1 - df_2)$ degrees of freedom.

So the *F*-statistic F:

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

Follows the *F-distribution* with $(df_1 - df_2)$ and df_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 sum of the *Explained Sum of Squares* (*ESS*) and the *Residual Sum of Squares* (*RSS*) is equal to the *Total Sum of Squares* (*TSS*):

$$TSS = ESS + RSS$$

A regression model that better explains the *response* data will have a larger *ESS* and a smaller *RSS*.

The *RSS* and the *ESS* follow independent *chi-squared* distributions with $(n-k)$ and $(k-1)$ degrees of freedom. Where k is the number of explanatory variables (including the intercept term).

The *F*-statistic of linear regression is equal to the ratio of the explained variance divided by the residual variance:

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

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

```
> # F-statistic from lm()
> 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] "Mean relative difference: 4.85e-07"
> # p-value of F-statistic
> 1-pf(q=fstat, df1=(ncols-1), df2=(nrows-ncols))
[1] 0.00757
```

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

A large value of the *F-statistic* indicates that the *ESS* is significantly greater than the *RSS*, and that the regression is able to explain the *response* data well.

A regression model that better explains the *response* data will have a larger *ESS* and a smaller *RSS*, so the *F-statistic* will be significantly greater than 1.

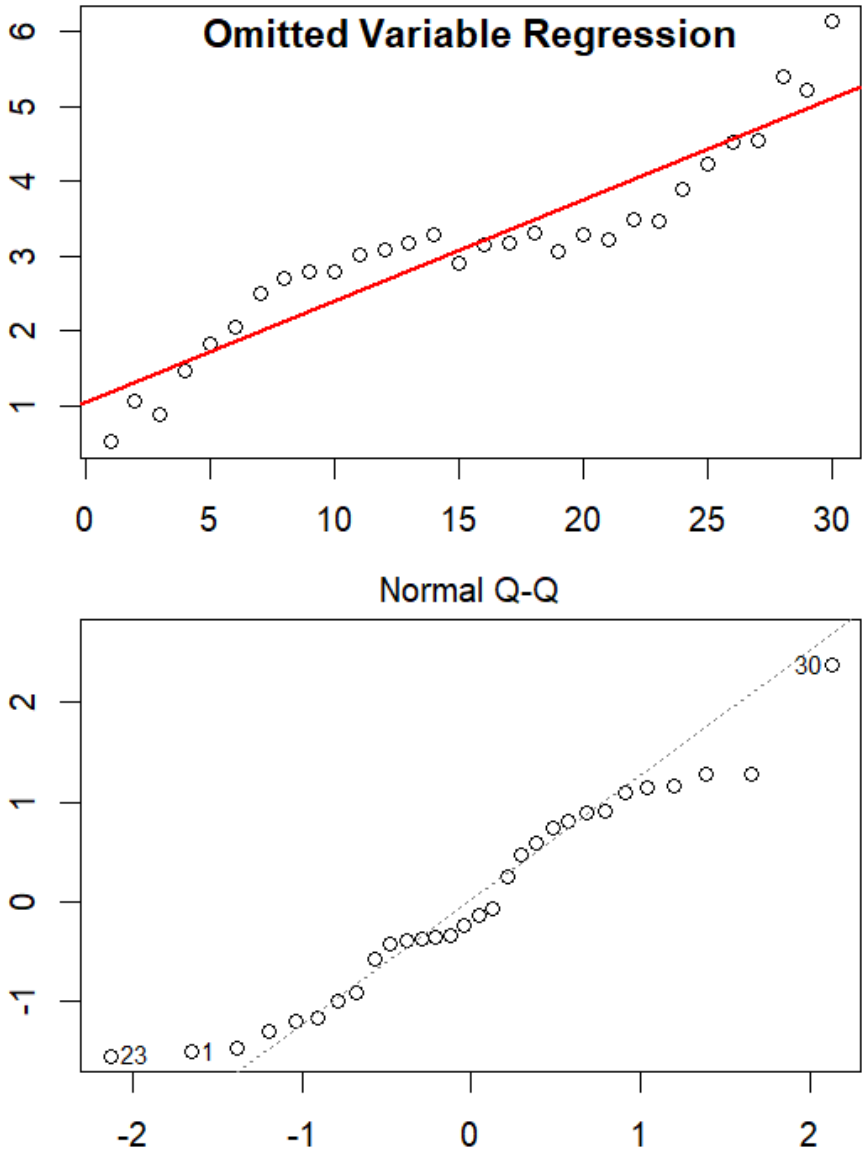
Omitted Variable Bias

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:

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

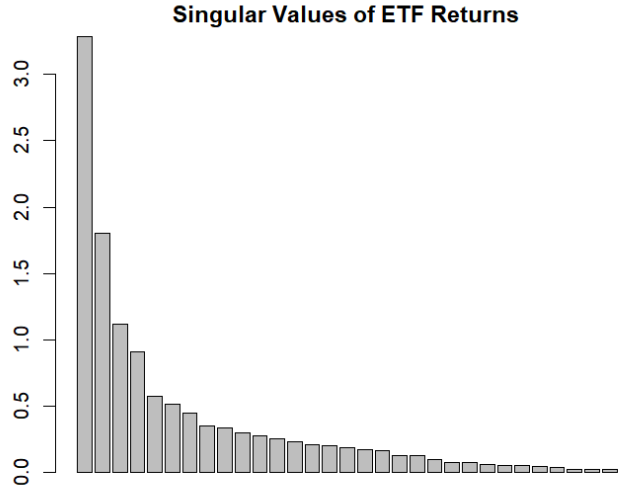
If any of the *singular values* are zero then the *generalized inverse* does not exist.

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$d)
> # Verify inverse property of the inverse
> all.equal(zoo::coredata(retp), retp %*% invmat %*% retp)
> # Calculate the regularized inverse from SVD
> dimax <- 1:3
> invreg <- svdec$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$rotation
> # Principal components are orthogonal to each other
> round(t(predpca) %*% predpca, 2)
> # Calculate the PCA influence matrix
> infmat <- predm %*% MASS::ginv(predm)
> infpca <- predpca %*% MASS::ginv(predpca)
> all.equal(infmat, infpca)
> # Calculate the regression coefficients
> betav <- drop(MASS::ginv(predm) %*% respv)
> # Transform the collinear regression coefficients to the PCA
> drop(betav %*% pcad$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 eigenvalues.

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
> betav <- drop(MASS::ginv(predcol) %*% respv)
> betav
> # Calculate the PCA predictors
> pcad <- prcomp(predcol, center=FALSE, scale=FALSE)
> predpca <- predcol %*% pcad$rotation
> round(t(predpca) %*% predpca, 6)
> # Transform the collinear regression coefficients to the PCA
> drop(betav %*% pcad$rotation)
> # Calculate the PCA regression coefficients
> betapca <- 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(betapca %*% MASS::ginv(pcad$rotation))
> betav
> # Calculate the regression coefficients after dimension reduction
> npca <- NROW(betapca)
> drop(betapca[-npca] %*% MASS::ginv(pcad$rotation)[-npca, ])
> # Compare with the collinear regression coefficients
> betav
> # Calculate the original regression coefficients
> drop(MASS::ginv(predm) %*% respv)
```

Ridge Regularized Regression

The objective function of *ridge regression* is equal to the *Residual Sum of Squares* (*RSS*) plus a penalty term proportional to the sum of squares of the coefficients:

$$O(\beta) = (y - \mathbb{X}\boldsymbol{\beta})^T (y - \mathbb{X}\boldsymbol{\beta}) + \lambda \sum_{i=1}^{n} \beta_i^2$$

Where λ is the regularization intensity parameter.

The *ridge regression* coefficients can be calculated using matrix inversion as follows:

$$\beta_{ridge} = (\mathbb{X}^T\mathbb{X} + \lambda\mathbb{1})^{-1}\mathbb{X}^T y = \mathbb{X}_\lambda^{-2}\mathbb{X}^T y$$

With $\mathbb{X}_\lambda^{-2} = (\mathbb{X}^T\mathbb{X} + \lambda\mathbb{1})^{-1}$.

```
> # Calculate the RRS and the penalty terms
> rrs <- sum((respv - predm %*% betar)^2)
> penalty <- lambdaf*sum(betar^2)
> c(RSS=rrs, Penalty=penalty, Objective=rrs + penalty)
> # Calculate the ridge objective function:
> ridgeobj <- function(respv, predm, betav, lambdaf) {
+   rrs <- sum((respv - predm %*% betav)^2)
+   penalty <- lambdaf*sum(betav^2)
+   residv <- respv - predm %*% betav
+   return(rrs + penalty)
+ } # end ridgeobj
> # Calculate ridge coefficients by minimizing ridge objective
> optiml <- optim(par=rep(0, NCOL(predm)),
+         ridgeobj,
+         respv=respv, predm=predm, lambdaf=lambdaf,
+         method="BFGS")
> optiml$par
> all.equal(optiml$par, betar, check.attributes=FALSE)
```

```
> # Regress the EEM returns on the other ETF returns
> predm <- na.omit(rutils::etfenv$returns[, c("SPY", "TLT", "USO", "XLB", "DBC", "EEM")])
> # Standardized the predictors
> predm <- scale(predm)
> respv <- predm[, "EEM"]
> predm <- predm[, -which(colnames(predm) == "EEM")]
> # Calculate the standard regression coefficients
> betav <- drop(MASS::ginv(predm) %*% respv)
> names(betav) <- colnames(predm)
> # Calculate the ridge regression coefficients
> lambdaf <- 1000
> unitmat<- diag(ncol(predm))
> betar <- drop(MASS::ginv(t(predm) %*% predm + lambdaf*unitmat) %*% t(predm) %*% respv)
> names(betar) <- colnames(predm)
```

Ridge Regression Coefficients

Ridge regression shrinks the less significant coefficients towards zero, but it does not set any of them exactly to zero.

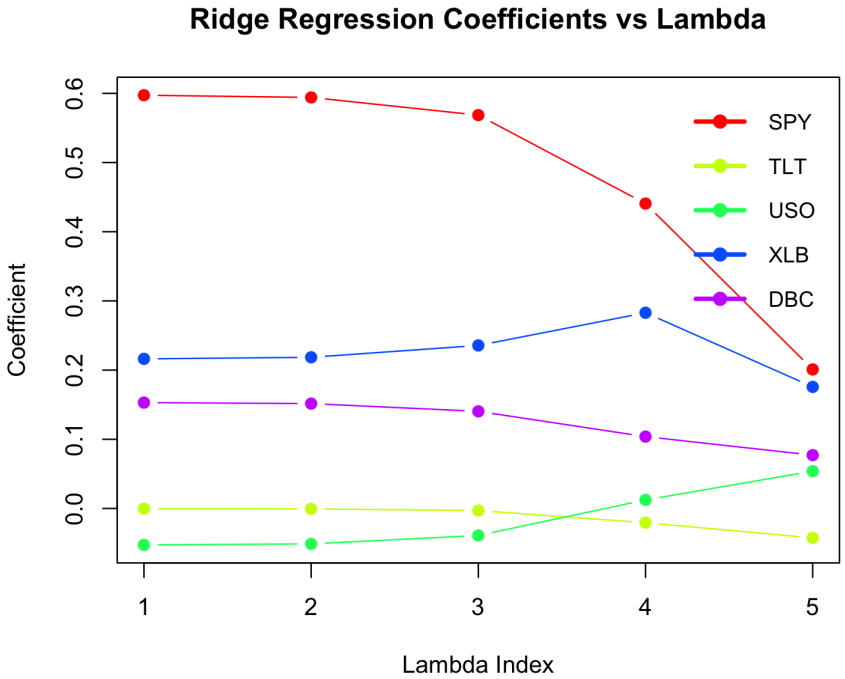
As the *regularization* intensity parameter λ becomes very large, the *ridge* coefficients tend to zero:

$$\lambda \to \infty \quad \Rightarrow \quad \beta_{ridge} \to \frac{1}{\lambda}\mathbb{X}^T y$$

When λ is very large, all the *ridge* coefficients tend to zero.

When λ is zero, the *ridge* coefficients are equal to the standard regression coefficients.

```
> # Calculate ridge coefficients for different lambda values
> lambdav <- c(0, 10, 100, 1000, 10000)
> coeffm <- sapply(lambdav, function(lambdaf) {
+   drop(MASS::ginv(t(predm) %*% predm + lambdaf*unitmat) %*% t(prec
+ }) ## end sapply
> rownames(coeffm) <- colnames(predm)
> colnames(coeffm) <- paste("lambda", lambdav, sep="=")
> round(coeffm, 4)
> # Plot ridge regression coefficients vs lambda with colors
> colorv <- rainbow(nrow(coeffm))
> matplot(t(coeffm), type="b", pch=19, lty=1, col=colorv,
+   main="Ridge Regression Coefficients vs Lambda",
+   xlab="Lambda intensity", ylab="Coefficient")
> legend("topright", legend=rownames(coeffm), lwd=3,
+   pch=19, lty=1, bty="n", col=colorv, cex=0.9)
```



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* $\mathbb{X}$.

```
> # Calculate the fitted values and the residuals
> fitv <- drop(predm %*% betav)
> residv <- drop(respv - fitv)
> # Inverse of the squared predictor matrix
> pred2 <- crossprod(predm)
> predinv <- MASS::ginv(pred2)
> # Calculate the variance of residuals
> degf <- (NROW(predm) - NCOL(predm))
> residvd <- sum(residv^2)/degf
> # Calculate the covariance matrix of betas
> covm <- residvd*predinv
```

Solution of Regression Using Coordinate Descent

Multivariate regression can also be solved recursively using *coordinate descent*:

$$r_j = y - \sum_{i \neq j} \beta_i x_i = y - \mathbb{X}_{-j} \beta_{-j}$$

$$\beta_j = \frac{x_j r_j}{x_j^T x_j}$$

The *partial residual* r_j is first calculated without the effect of the j-th *predictor*.

Then the updated *coefficient* β_j is equal to the projection of the *partial residual* r_j onto the j-th *predictor* vector x_j divided by the sum of squared *predictor* vector x_j.

The recursion is repeated until the *regression coefficients* β converge.

```
> # Solve multivariate regression using coordinate descent
> solve_cd <- function(respv, predm, maxit = 1000, tol = 1e-6) {
+   # Initialize the variables
+   ncols <- NCOL(predm)
+   colsq <- colSums(predm^2)
+   betav <- rep(0, ncols)
+   # Loop over iterations
+   for (iter in 1:maxit) {
+     betap <- betav
+     # Loop over the predictors
+     for (j in 1:ncols) {
+       # Calculate the partial residual excluding current predictor
+       residv <- respv - predm[, -j] %*% betav[-j]
+       # Calculate the product of predictor j with the residual
+       covp <- sum(predm[, j] * residv)
+       # Update beta_j coefficient
+       betav[j] <- covp / colsq[j]
+     } # end for j
+     # Break when converged
+     if (sum(abs(betav - betap)) < tol) break
+   } # end for iter
+   return(betav)
+ } # end solve_cd
> # Calculate the regression coefficients using coordinate descent
> betav <- solve_cd(respv, predm)
> all.equal(betav, drop(betac), check.attributes=FALSE)
[1] "Mean relative difference: 6.12e-07"
```

LASSO Regularized Regression

The objective function of *LASSO regression* is equal to the *RSS* plus a penalty term proportional to the sum of the absolute values of the coefficients:

$$O(\beta) = (y - \mathbb{X}\beta)^T (y - \mathbb{X}\beta) + \lambda \sum_{i=1}^{n} |\beta_i|$$

Where λ is the regularization intensity parameter.

The *LASSO regression* coefficients can be calculated using *coordinate descent* with soft-thresholding:

$$r_j = y - \sum_{i \neq j} \beta_i x_i = y - \mathbb{X}_{-j} \beta_{-j}$$

$$c_j = x_j r_j$$

$$c_j = sign(c_j)\, max(|c_j| - \lambda, 0)$$

$$\beta_j = \frac{c_j}{x_j^T x_j}$$

The *partial residual* r_j is calculated without the effect of the j-th *predictor*.

Soft-thresholding is applied to the projection c_j of the *partial residual* r_j onto the j-th *predictor* vector x_j.

The *coefficient* β_j is equal to the projection c_j divided by the sum of squared *predictor* vector x_j.

The recursion is repeated until the *regression coefficients* β converge.

```
> # Solve LASSO regression using coordinate descent
> solvelasso <- function(respv, predm, lambda, maxit = 1000, tol = 1
+   # Initialize the variables
+   nrows <- NROW(predm)
+   ncols <- NCOL(predm)
+   colsq <- colSums(predm^2) / nrows
+   betav <- rep(0, ncols)
+   # Loop over iterations
+   for (iter in 1:maxit) {
+     betap <- betav
+     # Loop over the predictors
+     for (j in 1:ncols) {
+       # Calculate the partial residual excluding current predictor
+       residv <- respv - predm[, -j] %*% betav[-j]
+       # Calculate the product of predictor j with the residual
+       covp <- sum(predm[, j] * residv) / nrows
+       # Apply soft-thresholding to the covariate
+       covp <- sign(covp) * max(abs(covp) - lambda, 0)
+       # Update beta_j coefficient
+       betav[j] <- covp / colsq[j]
+     } # end for j
+     # Break when converged
+     if (sum(abs(betav - betap)) < tol) break
+   } # end for iter
+   return(betav)
+ } # end solvelasso
> # Calculate the LASSO coefficients using coordinate descent
> betav <- solvelasso(respv, predm, lambda=0.0)
> all.equal(betav, drop(betac), check.attributes=FALSE)
```

The soft-thresholding shrinks the coefficients to zero if they are less than the regularization parameter λ.

Homework Assignment

Required

- Study all the lecture slides in *FRE6871_Lecture_3.pdf*, and run all the code in *FRE6871_Lecture_3.R*

Recommended

- Read about *optimization methods*:
  Bolker Optimization Methods.pdf, *Yollin Optimization.pdf*, *DEoptim Introduction.pdf*, *Boudt DEoptim Large Portfolio Optimization.pdf*.