Analysis of NIR data

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[1] "2012-06-13 23:45:19"
```

NIR measurements are made at 152 wavelengths on 17 milk samples. Milk runs trough a glass tube. **Near infra red** light is sent through the tube and the the amount of light that goes through the milk at different wavelengths is recorded. The milk is analyzed for contents of fat, lactose, protein and drymatter.

The question is whether fat,lactose, protein and drymatter can be predicted from the NIR measurements.

```
> data(NIRmilk, package = "doBy")

> dim(NIRmilk)

[1]  17 158

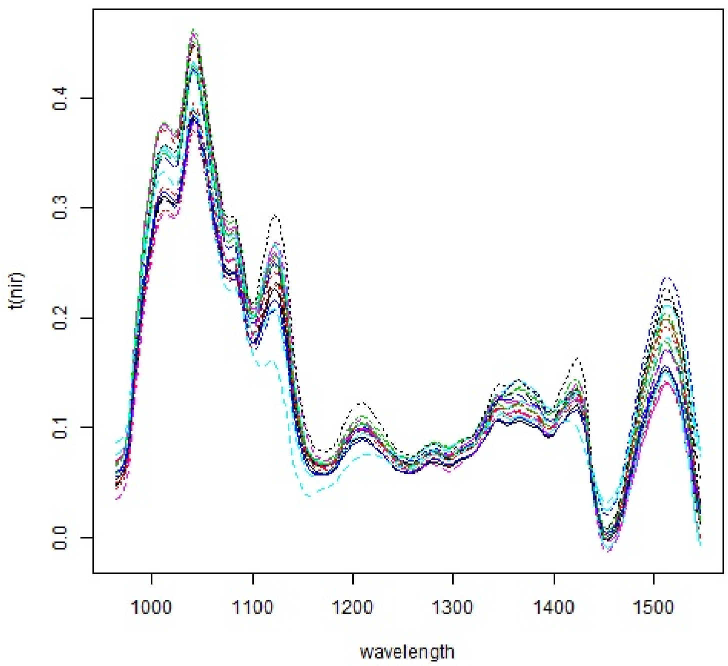
> head(round(NIRmilk[, c(1:6, 152:158)], 3))

  sample  X964  X968  X972  X976  X979 X1542 X1546  X1550   fat protein lactose
1      1 0.054 0.056 0.061 0.078 0.109 0.034 0.012 -0.008 4.168   3.639   4.530
2      2 0.069 0.071 0.078 0.098 0.135 0.022 0.000 -0.020 4.227   3.549   5.564
3      3 0.068 0.070 0.077 0.099 0.136 0.059 0.033  0.010 3.904   4.299   5.490
4      4 0.055 0.057 0.062 0.080 0.110 0.108 0.082  0.060 3.162   4.547   4.356
5      5 0.075 0.077 0.082 0.101 0.135 0.101 0.080  0.061 2.144   4.108   5.104
6      6 0.069 0.071 0.077 0.099 0.136 0.037 0.015 -0.004 4.352   3.413   5.626
      dm
1 13.067
2 14.063
3 14.470
4 12.893
5 12.127
6 14.177

> nir <- NIRmilk[, 2:153]

> waveLength <- gsub("\\.", "", (gsub("X", "", names(nir))))

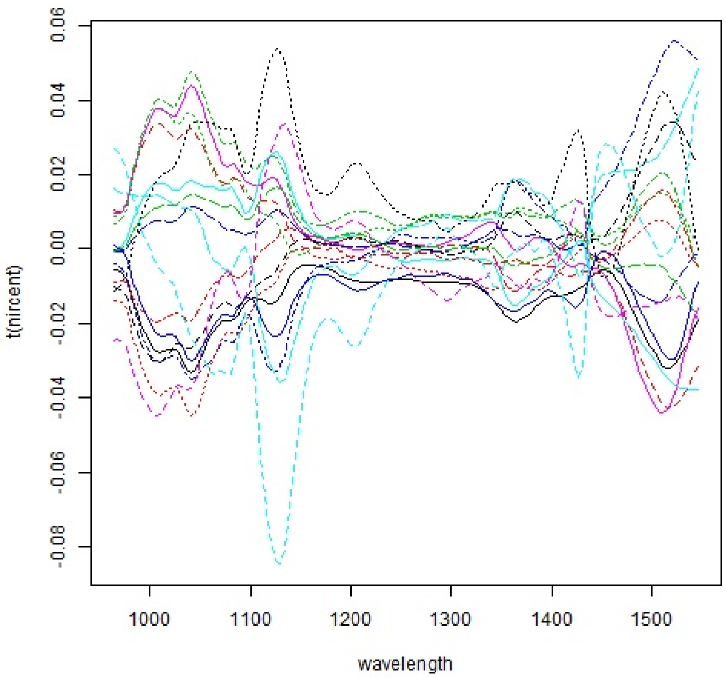
> matplot(waveLength, t(nir), type = "l", xlab = "wavelength")
```



More variation in data is revealed if data is centered around the mean of each column

```
> nircent <- scale(nir, center = TRUE, scale = FALSE)
```

```
> matplot(waveLength, t(nircent), type = "l", xlab = "wavelength")
```



We make a PCA on the centered data:

```
> PCA <- prcomp(nircent)

> summary(PCA)

Importance of components:
                          PC1    PC2     PC3     PC4      PC5      PC6      PC7
Standard deviation     0.1575 0.1202 0.09539 0.02046 0.004769 0.003699 0.002117
Proportion of Variance 0.5081 0.2959 0.18641 0.00858 0.000470 0.000280 0.000090
Cumulative Proportion  0.5081 0.8040 0.99043 0.99900 0.999470 0.999750 0.999840
                           PC8      PC9     PC10      PC11      PC12      PC13
Standard deviation     0.00174 0.001176 0.001104 0.0008254 0.0007399 0.0005534
Proportion of Variance 0.00006 0.000030 0.000020 0.0000100 0.0000100 0.0000100
Cumulative Proportion  0.99990 0.999930 0.999960 0.9999700 0.9999800 0.9999900
                            PC14      PC15      PC16      PC17
Standard deviation     0.0005226 0.0004632 0.0004033 1.092e-17
Proportion of Variance 0.0000100 0.0000000 0.0000000 0.000e+00
Cumulative Proportion  0.9999900 1.0000000 1.0000000 1.000e+00
```

Hence, 80 % of the total variation in a 150--dimensional data set is explained by the first two principal components and practically all variation is explained by the first three principal components. This is quite a substantial reduction in dimension.

We can display the loadings as

```
> matplot(waveLength, PCA$rot[, 1:3], type = "l", col = 1:3, lty = 1,

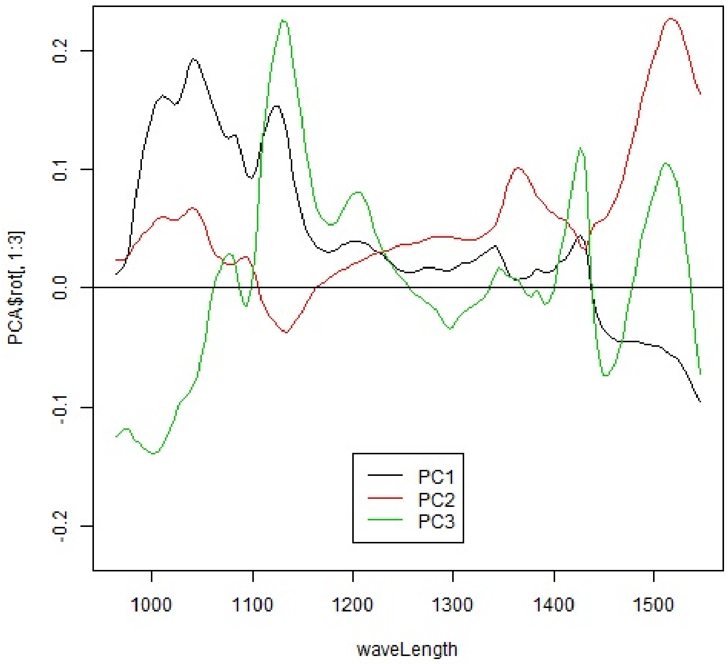
>     ylim = c(-0.22, 0.22))

> abline(h = 0)

> library(gplots)

> smartlegend("center", "bottom", legend = c("PC1", "PC2", "PC3"),

>     col = c(1:3), lty = c(1, 1, 1))
```



So - the loadings for PC1 (black line) come mainly from the low wavelengths; loadings for PC2 (red line) come mainly from high wavelengths loadings for PC3 come from, more localized regions of wavelengths. Finally the intermediate wavelengths seem to contribute only slightly to all three components.

PCR: Principal component regression

Principal component regression is very straight forward:

1. First derive principal components of the explanatory variables and
2. Then use these principal components as explanatory variables.

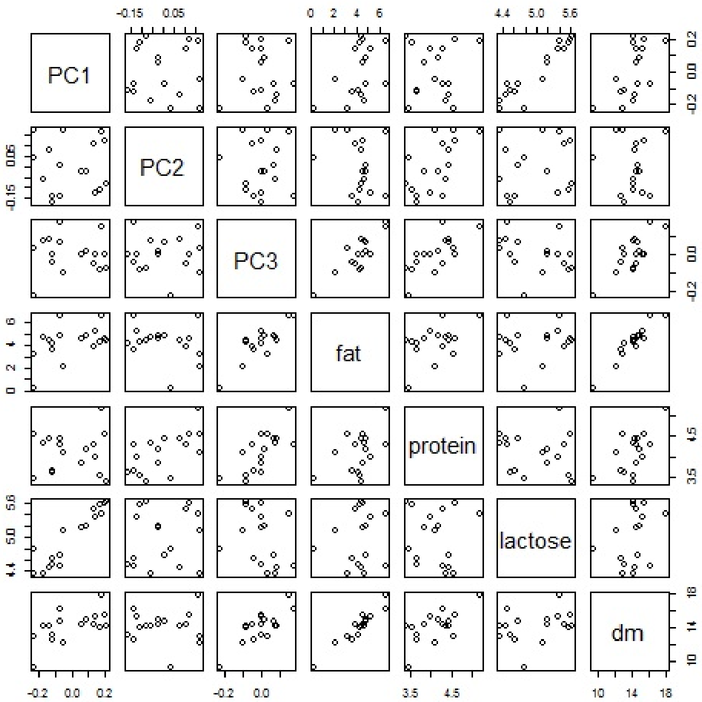
Let us combine the first three principal components with the responses:

```
> nirnew <- cbind(PCA$x[, 1:3], NIRmilk[, 155:158])

> head(nirnew)

          PC1         PC2          PC3    fat protein lactose      dm
1 -0.11594522 -0.17025096 -0.004671534 4.1683  3.6390  4.5300 13.0667
2  0.17489004 -0.11226120 -0.084292848 4.2273  3.5490  5.5643 14.0633
3  0.13820007  0.11101555 -0.047871832 3.9040  4.2993  5.4897 14.4700
4 -0.22655731  0.17527552  0.033194764 3.1617  4.5467  4.3560 12.8933
5 -0.05103537  0.17342919 -0.099546952 2.1443  4.1083  5.1037 12.1267
6  0.21445607 -0.08096041 -0.080089550 4.3520  3.4133  5.6257 14.1767

> pairs(nirnew)
```



Now, we can try to make a multiple regression explaining <u>fat</u> not directly in terms of the wavelengths but in terms of the principal components:

```
> m1 <- lm(fat ~ PC1 + PC2 + PC3, data = nirnew)

> summary(m1)


Call:
lm(formula = fat ~ PC1 + PC2 + PC3, data = nirnew)

Residuals:
      Min        1Q    Median        3Q       Max
-0.084584 -0.026316 -0.006242  0.034143  0.061544

Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept)  4.24592    0.01111  382.05  < 2e-16 ***
PC1          4.32000    0.07274   59.39  < 2e-16 ***
PC2         -3.07567    0.09532  -32.27 8.53e-14 ***
PC3         13.27432    0.12009  110.54  < 2e-16 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 0.04582 on 13 degrees of freedom
Multiple R-squared: 0.9992, Adjusted R-squared: 0.999
F-statistic:  5596 on 3 and 13 DF,  p-value: < 2.2e-16
```