Analysis of High Dimensional Data

Homework 1

21 Feb 2016

```
# First set your working directory (with data file CanadianWeather.rda),
#     and install the required packages
#setwd("~/dropbox/education/AnalysisHighDimensionalData/Homeworks1516/")
#install.packages("ldr")
```

This text contains an introduction to the data and to Functional Data Analysis. The details of the assingment can be found at the end of this text.

1. Introduction

1.1. Data

We have data on avarage daily rainfall (mm/day) for the 365 days in the year and for 35 Canadian cities.

First we read the data

```
load("CanadianWeather.rda")

da<-CanadianWeather[[1]]
da<-da[,,"Precipitation.mm"] # precipitation data
head(da)
```

```
##       St. Johns Halifax Sydney Yarmouth Charlottvl Fredericton Scheffervll
## jan01       5.2     6.0    5.3      5.6        4.6         4.0         1.1
## jan02       5.8     5.3    5.2      3.7        4.4         3.2         1.3
## jan03       3.9     2.6    2.1      2.8        2.3         3.3         1.2
## jan04       4.3     5.3    5.0      5.3        4.8         3.3         1.3
## jan05       6.2     6.0    7.3      3.8        5.1         2.7         1.0
## jan06       3.4     2.1    2.2      2.4        1.5         0.8         1.3
##       Arvida Bagottville Quebec Sherbrooke Montreal Ottawa Toronto London
## jan01    2.6         3.0    4.1        2.9      2.9    2.5     1.8    2.4
## jan02    1.2         1.8    2.3        2.9      1.2    1.1     0.9    1.4
## jan03    2.1         1.3    2.6        1.9      1.4    1.3     0.9    1.8
## jan04    2.3         2.5    4.3        2.9      3.6    3.1     1.5    2.9
## jan05    1.7         2.1    2.3        2.1      1.6    1.3     0.8    1.1
## jan06    2.0         1.6    1.5        0.8      1.1    1.3     1.0    1.4
##       Thunder Bay Winnipeg The Pas Churchill Regina Pr. Albert
## jan01         0.7      0.5     0.5       0.5    0.2        0.1
## jan02         1.9      0.6     0.9       0.6    0.3        0.9
## jan03         0.8      0.3     0.7       0.5    0.6        0.6
## jan04         0.3      0.5     0.5       0.4    0.3        0.3
## jan05         0.8      0.4     0.2       0.4    0.8        0.2
## jan06         1.7      0.7     0.9       0.2    0.5        0.3
##       Uranium City Edmonton Calgary Kamloops Vancouver Victoria Pr. George
## jan01          0.3      0.4     0.3      0.6       5.5      5.3        2.2
```

```
## jan02          0.4      0.8     0.1      0.4       6.6      5.2        1.9
## jan03          1.3      1.1     0.3      1.2       6.8      5.4        1.9
## jan04          0.6      1.1     0.6      1.3       5.1      4.5        1.8
## jan05          0.8      1.0     1.0      1.2       3.8      4.6        1.1
## jan06          1.1      0.8     0.2      0.5       2.5      2.6        1.2
##       Pr. Rupert Whitehorse Dawson Yellowknife Iqaluit Inuvik Resolute
## jan01        6.0        0.5    0.9         0.6     1.1    0.8      0.1
## jan02        5.0        0.8    0.6         0.7     0.9    0.9      0.1
## jan03        6.7        1.1    0.8         0.3     0.8    0.8      0.0
## jan04        7.1        0.2    0.8         0.5     0.7    0.4      0.2
## jan05        6.1        0.6    1.0         0.7     0.9    0.8      0.2
## jan06        8.1        0.7    1.0         0.5     0.2    0.4      0.2
```

Here is a list of the 35 cities

```r
colnames(da)
```

```
##  [1] "St. Johns"    "Halifax"      "Sydney"       "Yarmouth"
##  [5] "Charlottvl"   "Fredericton"  "Scheffervll"  "Arvida"
##  [9] "Bagottville"  "Quebec"       "Sherbrooke"   "Montreal"
## [13] "Ottawa"       "Toronto"      "London"       "Thunder Bay"
## [17] "Winnipeg"     "The Pas"      "Churchill"    "Regina"
## [21] "Pr. Albert"   "Uranium City" "Edmonton"     "Calgary"
## [25] "Kamloops"     "Vancouver"    "Victoria"     "Pr. George"
## [29] "Pr. Rupert"   "Whitehorse"   "Dawson"       "Yellowknife"
## [33] "Iqaluit"      "Inuvik"       "Resolute"
```

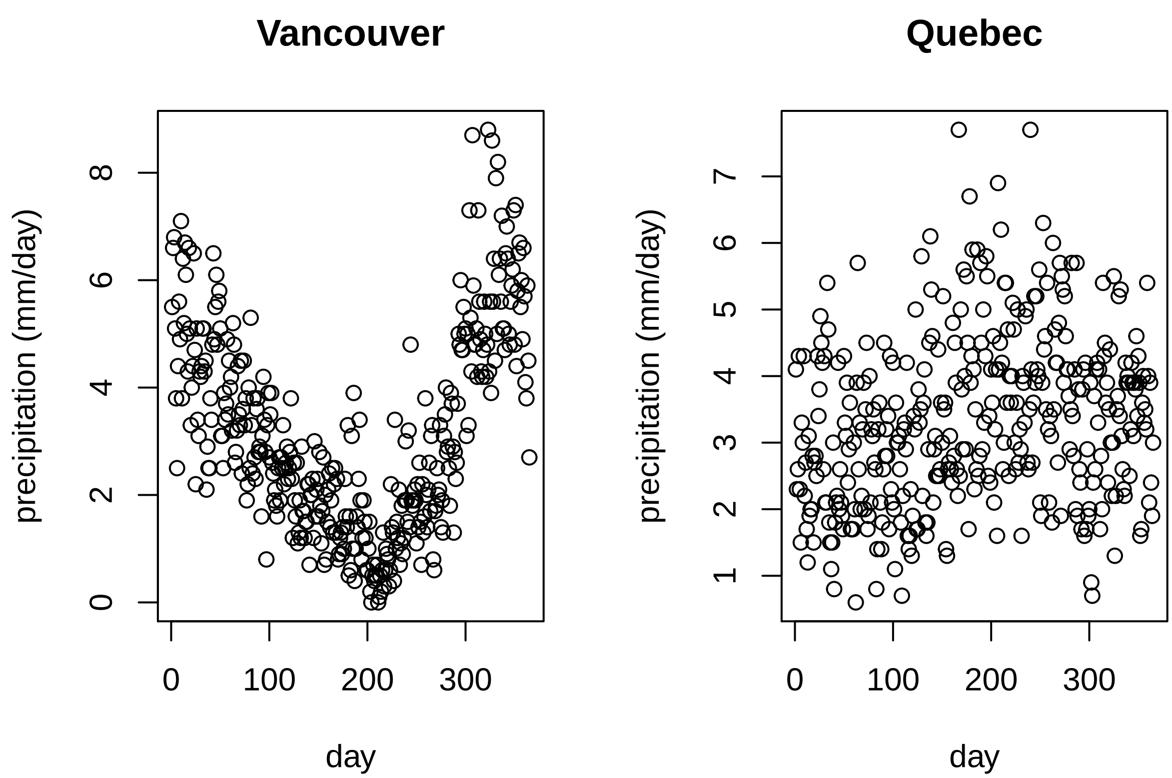
The data set also contains extra information about the cities. For example, the regions, provinces and the coordinates are included.

```r
MetaData<-data.frame(city=colnames(da), region=CanadianWeather$region, province=CanadianWeather$provinc
head(MetaData)
```

```
##                    city   region      province coord.N.latitude
## St. Johns     St. Johns Atlantic  Newfoundland            47.34
## Halifax         Halifax Atlantic   Nova Scotia            44.39
## Sydney           Sydney Atlantic   Nova Scotia            46.09
## Yarmouth       Yarmouth Atlantic   Nova Scotia            43.50
## Charlottvl   Charlottvl Atlantic       Ontario            42.48
## Fredericton Fredericton Atlantic New Brunswick            45.58
##             coord.W.longitude
## St. Johns               52.43
## Halifax                 63.36
## Sydney                  60.11
## Yarmouth                66.07
## Charlottvl              80.25
## Fredericton             66.39
```

I show you the data of Vancouver and Quebec.

```r
par(mfrow=c(1,2))
plot(1:365,da[,"Vancouver"], main="Vancouver", xlab="day", ylab="precipitation (mm/day)")
plot(1:365,da[,"Quebec"], main="Quebec", xlab="day", ylab="precipitation (mm/day)")
```




```r
par(mfrow=c(1,1))
```

1.2. Research Question

The objective is to discover which cities have similar precipitation patterns, and which have dissimilar patterns. We need a 2-dimensional graph that shows each city as a point, such that cities with similar precipitation patters are close to one another. We also want to understand the difference in rainfall patterns: in what sense do they differ (e.g overall more rainfall in Western Canada, or less rain in summer, . . .).

1.3. Functional Data Analysis

1.3.1. Introduction

From the research question we conclude that a MDS is an appropriate method.

On way of looking at the data is to consider it as a multivariate data set with $n = 35$ rows (cities) and $p = 365$ columns (days). However, this is not the approach that we take. In this section I will introduce a functional data analysis (FDA) approach.

In FDA we typically consider functions as observations. For example, for each of the 35 cities we have observations on a precipitation function. To take this approach it is necessary for each city to first convert the 365 data entries to a single function. This function will contain parameter estimates (typically less than the original number of data entries, say $q < p = 365$). Thus each city will have its set of q parameter estimates, and thus an $n \times q$ data matrix can be constructed. These parameter estimates form now the input for the MDS. To give a meaningful interpretation to the results, at the end we need to back-transform our solution from the parameter space to the function space.

1.3.2. Transformation to functions

Let $Y_i(t)$ denote the outcome of observation $i = 1, \ldots, n$ (here: average daily rainfall) at time $t \in [1, 365]$. For observation i we have data on times t_{ij}, $j = 1, \ldots, p_i$. This setting thus allows for irregularly spaces measurements: each observation i may come with its own set of time points t_{ij} with measurements $Y_i(t_{ij})$. Our data set, however, contains regularly spaced data: for each city i precipitations are available for $t = 1, 2, \ldots, 365$.

Consider the non-linear statistical model

$$Y_i(t_{ij}) = f_i(t_{ij}) + \varepsilon_{ij} \quad i = 1, \ldots, n; j = 1, \ldots, p_i$$

for some smooth functions $f_i(\cdot)$ and with ε_{ij} i.i.d. with mean 0 and constant variance σ^2. If $f_i(\cdot)$ is a parametric function, then non-linear least squares can be used to estimate the parameters.

Functional approximation theory (mathematical theory) says that a sufficiently smooth function $f(\cdot)$ can be arbitrary well approximated by the expansion

$$f_i(t) = \sum_{k=0}^{\infty} \theta_{ik} \phi_k(t)$$

where the θ_{ik} are parameters, and the $\phi_k(\cdot)$ form an set of orthonormal basis functions. In practice the expansion (sum) is truncated after a few terms, say m. For this homework it is not important to exactly understand the meaning of an orthonormal basis. Classical examples of orthonormal basis functions: Fourier functions, polynomial basis functions, wavelet functions. For this homework you may choose between a Fourier or a polynomial basis.

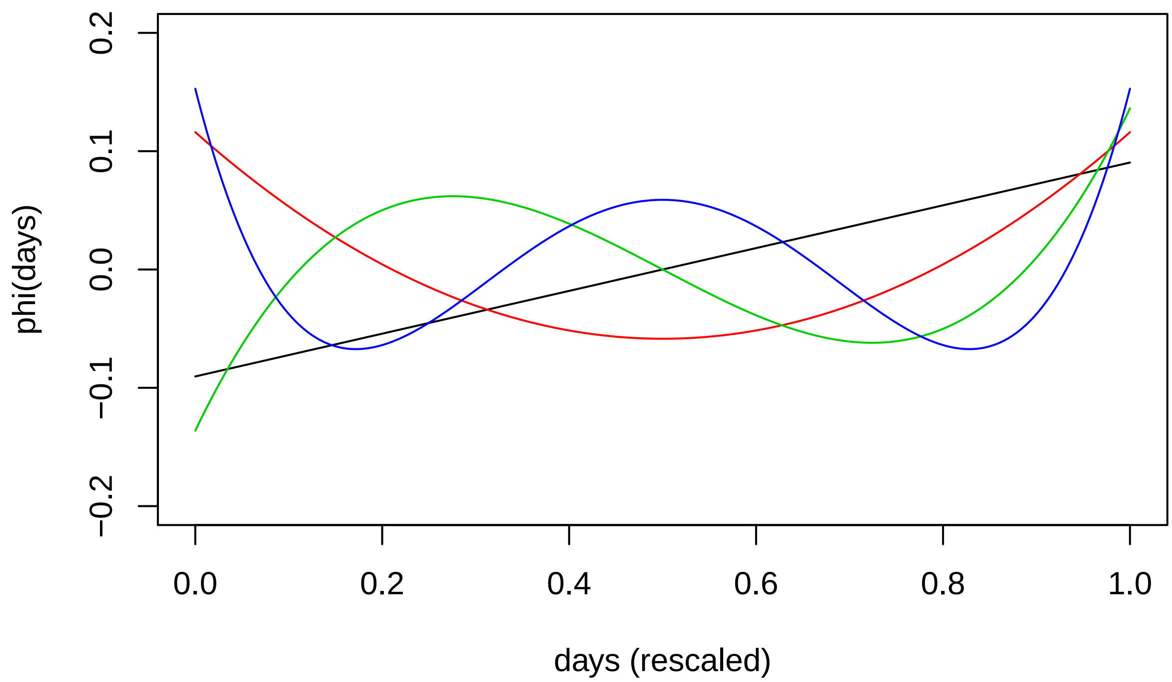
Functions from a polynomial basis are of the form

$$\phi_k(t) = \sum_{j=0}^{k} \alpha_j t^j,$$

i.e. $\phi_k(\cdot)$ is a polynomial function in t of degree k. The α_j's are constants (no need to estimate).

The next chunck of R code illustrates the generation of a polynomial basis. Note that I rescaled the 365 days to the $[0, 1]$ interval. This is only to avoid numerical problems when computing days^j for a large j.

```
days<-1:365
days<-(days-min(days))/(diff(range(days))) # rescaling to [0,1]
phi<-poly(days,degree=4)
# the i-th column of phi contains the i-th order
#    polynomial evaluated in "days"

plot(days,phi[,1],type="l",ylim=c(-0.2,0.2), xlab="days (rescaled)", ylab="phi(days)")
lines(days,phi[,2],type="l",col=2)
lines(days,phi[,3],type="l",col=3)
lines(days,phi[,4],type="l",col=4)
```




```
# the next line demonstrates that the polynomials are normalised
#    (no need to exactly understand this)
colMeans(scale(phi,center=T,scale=F)^2)
```

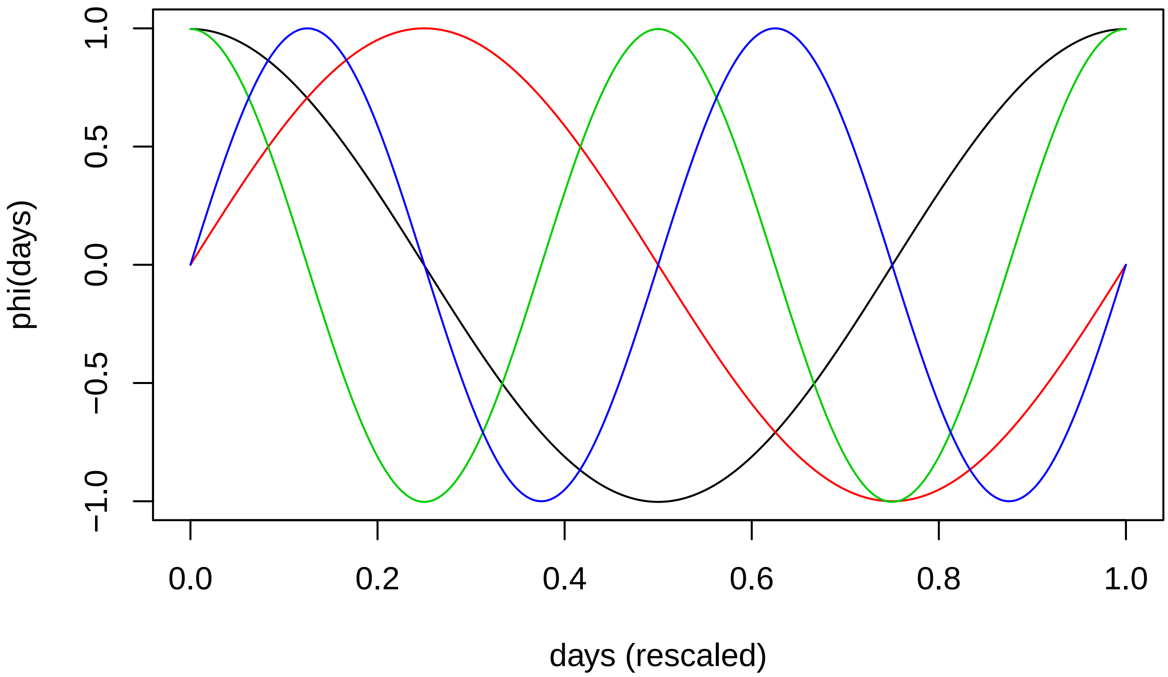
```
##           1           2           3           4
## 0.002739726 0.002739726 0.002739726 0.002739726
```

Now an exampel with the Fourier basis.

```
library(ldr) # needed for the bf function for generation of Fourier basis
```

```
## Loading required package: GrassmannOptim
## Loading required package: Matrix
```

```
phi<-bf(days,case="fourier",degree=4)
# the i-th column of phi contains the i-th order
#    Fourier basis function evaluated in "days"

plot(days,phi[,1],type="l",ylim=c(-1,1), xlab="days (rescaled)", ylab="phi(days)")
lines(days,phi[,2],type="l",col=2)
lines(days,phi[,3],type="l",col=3)
lines(days,phi[,4],type="l",col=4)
```




```r
# the next line demonstrates that the polynomials are normalised
#    (no need to exactly understand this)
colMeans(scale(phi,center=T,scale=F)^2)
```

```
## [1] 0.5013624 0.4986301 0.5013624 0.4986301 0.5013624 0.4986301 0.5013624
## [8] 0.4986301
```

The R code has demonstrated that the poly and bf functions transform a vector with the days at which measurements are available, to a matrix. For a given city (i.e. for a given i), the number of rows of the matrix equals the number of days, and each column corresponds to a basis function. The (j, k)th element of the matrix equals the kth basis function evaluated in the jth day t_{ij}. Let $x_{ijk} = \phi_k(t_{ij})$ denote this element.

We now rewrite the statistical model for $Y_i(t_{ij})$,

$$Y_i(t_{ij}) = \sum_{k=0}^{m} \theta_{ik}\phi_k(t_{ij}) + \varepsilon_{ij}$$

or

$$Y_i(t_{ij}) = \sum_{k=0}^{m} \theta_{ik}x_{ijk} + \varepsilon_{ij}.$$

For a given i, this has the structure of a linear regression model with outcomes $Y_i(t_{ij})$, $j = 1, \ldots, n$, and $q = m + 1$ regressors x_{ijk}.

Finally, we write the statistical model for city i in matrix notation.

$$\boldsymbol{Y}_i = \boldsymbol{\theta}_i^t \boldsymbol{X}_i + \boldsymbol{\varepsilon}_i$$

with $\boldsymbol{Y}_i$ the vector with the outcomes of observation i (one for each day t_{ij}), $\boldsymbol{\theta}_i$ the vector with the θ_{ik} (one for each basis function k), $\boldsymbol{X}_i$ the matrix with the x_{ijk} (days j in the rows, basis function index k in columns), and $\boldsymbol{\varepsilon}_i$ the vector with the i.i.d. error terms.

The parameters θ_{ik} can be estimated by means of least squares. This is illustrated in the next R code for a single city (i.e. a single i). The process need to be repeated for all cities $i = 1, \ldots, n$. Once the parameters are estimated they can be used to plot the fitted function.

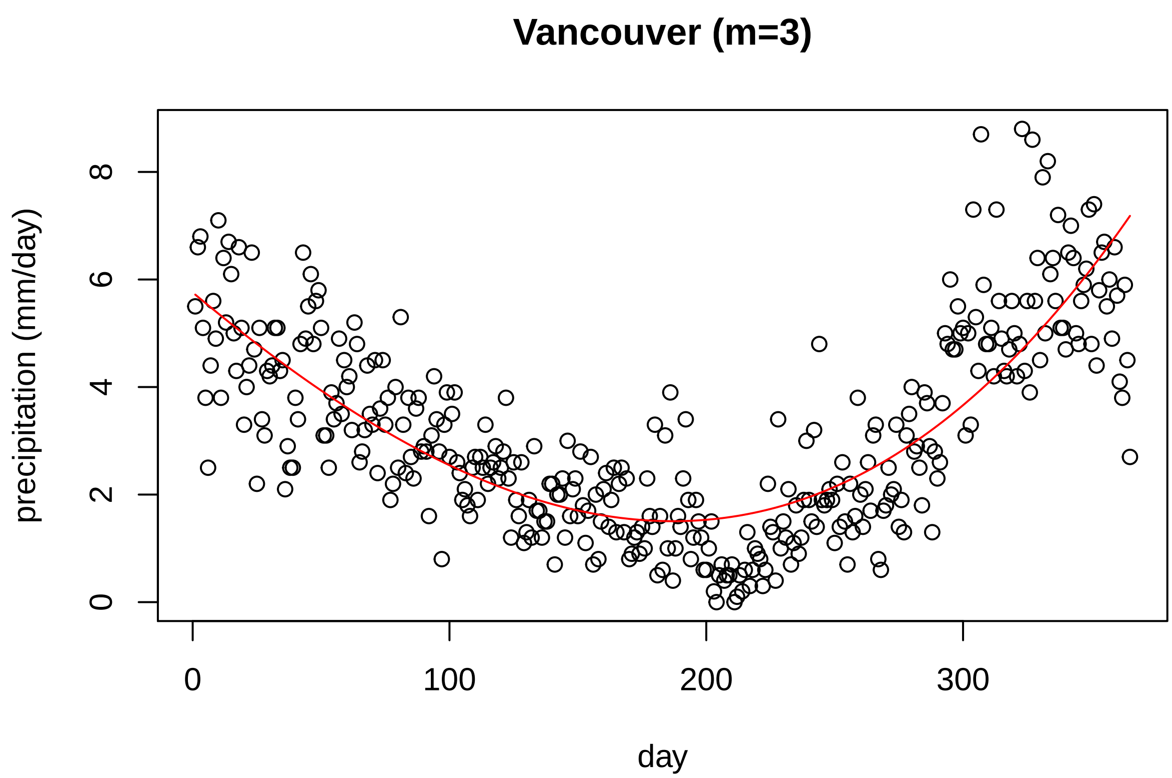
```
# Using the polynomial basis functions up to degree 3

days<-1:365
days<-(days-min(days))/(diff(range(days))) # rescaling to [0,1]
phi<-poly(days,degree=3)
dim(phi)
```

```
## [1] 365   3
```

```
# estimation of the theta parameters for Vancouver
m.Vancouver<-lm(da[,"Vancouver"]~phi)
summary(m.Vancouver)
```

```
##
## Call:
## lm(formula = da[, "Vancouver"] ~ phi)
##
## Residuals:
##     Min      1Q  Median      3Q     Max
## -4.4831 -0.7312 -0.1068  0.6815  4.7459
##
## Coefficients:
##             Estimate Std. Error t value Pr(>|t|)
## (Intercept)   3.1647     0.0592  53.455  < 2e-16 ***
## phi1          3.9234     1.1311   3.469 0.000586 ***
## phi2         28.3115     1.1311  25.031  < 2e-16 ***
## phi3          2.7691     1.1311   2.448 0.014833 *
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 1.131 on 361 degrees of freedom
## Multiple R-squared:  0.641,  Adjusted R-squared:  0.638
## F-statistic: 214.9 on 3 and 361 DF,  p-value: < 2.2e-16
```

```
# plot of fitted function
plot(1:365,da[,"Vancouver"],main="Vancouver (m=3)" ,xlab="day", ylab="precipitation (mm/day)")
lines(1:365,m.Vancouver$fitted.values,type="l", col=2)
```




```
# Using the polynomial basis functions up to degree 10

days<-1:365
days<-(days-min(days))/(diff(range(days))) # rescaling to [0,1]
phi<-poly(days,degree=10)
dim(phi)
```

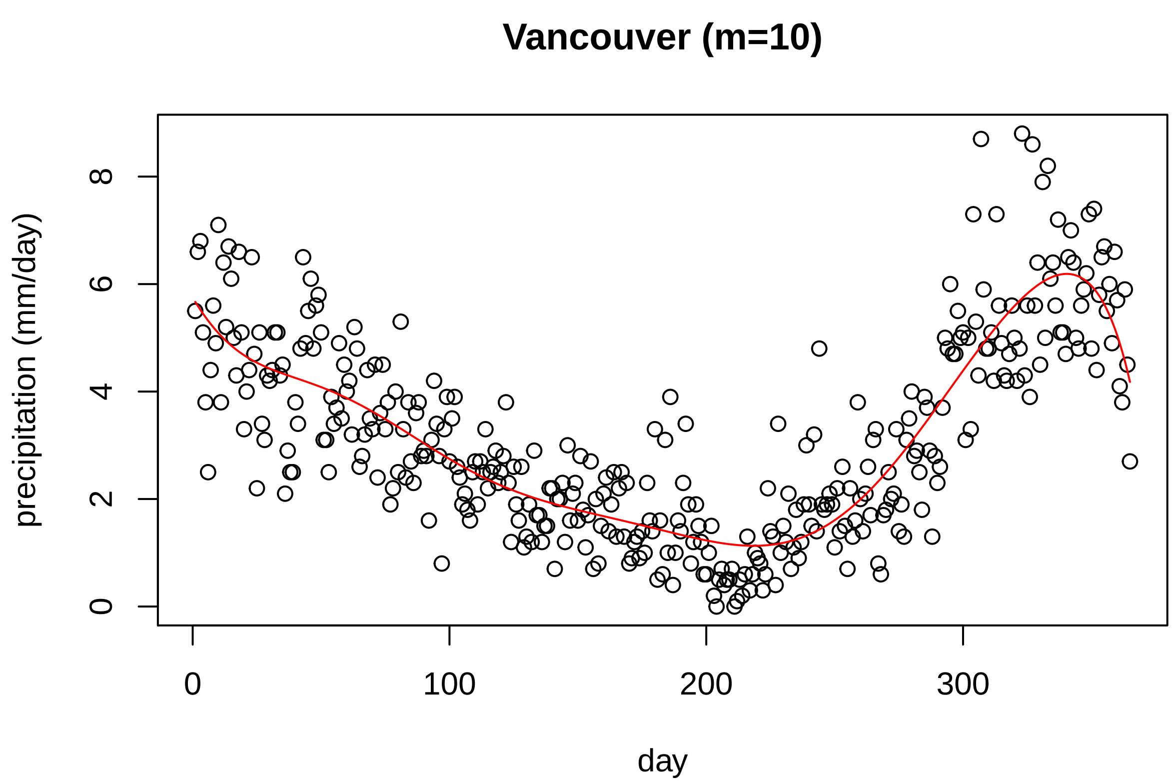
```
## [1] 365  10
```

```
# estimation of the theta parameters for Vancouver
m.Vancouver<-lm(da[,"Vancouver"]~phi)
summary(m.Vancouver)
```

```
##
## Call:
## lm(formula = da[, "Vancouver"] ~ phi)
##
## Residuals:
##     Min      1Q  Median      3Q     Max
## -2.8201 -0.6551 -0.0621  0.5794  3.8571
##
## Coefficients:
##              Estimate Std. Error t value Pr(>|t|)
## (Intercept)    3.1647     0.0523  60.511  < 2e-16 ***
## phi1           3.9234     0.9992   3.927 0.000104 ***
```

```
## phi2         28.3115     0.9992  28.335  < 2e-16 ***
## phi3          2.7691     0.9992   2.771 0.005878 **
## phi4         -6.7529     0.9992  -6.758 5.76e-11 ***
## phi5         -6.9005     0.9992  -6.906 2.32e-11 ***
## phi6         -3.4009     0.9992  -3.404 0.000741 ***
## phi7         -1.2774     0.9992  -1.278 0.201913
## phi8          1.2035     0.9992   1.205 0.229201
## phi9         -0.4364     0.9992  -0.437 0.662548
## phi10        -0.6000     0.9992  -0.601 0.548537
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 0.9992 on 354 degrees of freedom
## Multiple R-squared:  0.7253, Adjusted R-squared:  0.7175
## F-statistic: 93.46 on 10 and 354 DF,  p-value: < 2.2e-16
```

```r
# plot of fitted function
plot(1:365,da[,"Vancouver"],main="Vancouver (m=10)", xlab="day", ylab="precipitation (mm/day)")
lines(1:365,m.Vancouver$fitted.values,type="l", col=2)
```



The R code demonstrate that the quality of the fit improves with increasing number of basis functions. Later in the course we will see methods for choosing an appropriate number of basis functions. For this homework I suggest that you choose an $m \leq 20$ that makes sense to you. I'm not claiming that this is a good method, but for now this will do.

1.3.3. Multidimensional Scaling of Functions

Let $\hat{\boldsymbol{\theta}}_i$ denote the vector with the parameter estimates. Given the set of basis functions, $\hat{\boldsymbol{\theta}}_i$ contain the information (shape) of the precipitation functions for observation i. The estimates for all cities can be collected into a single new $n \times (m+1)$ data matrix $\boldsymbol{\Theta}$. The ith row of $\boldsymbol{\Theta}$ is $\hat{\boldsymbol{\theta}}_i^t$. The matrix $\boldsymbol{\Theta}$ contains now all information on the shape of the precipitation functions. Since $\boldsymbol{\Theta}$ has the structure of an ordinal data matrix, classical multivariate techniques can be applied to it. We will apply a MDS to $\boldsymbol{\Theta}$, so that we can construct a 2-dimensional plot with each point representing a city. The distances between the points in the 2-dimensional MDS space are approximations of the distances between the rows of $\boldsymbol{\Theta}$, and hence can be interpreted as distances between the precipitation functions.

The MDS thus starts from the truncated SVD of $\boldsymbol{\Theta}$,

$$\boldsymbol{\Theta}_k = \boldsymbol{U}_k \boldsymbol{D}_k \boldsymbol{V}_k^t$$

(note that the index k now refers to the number of components in the truncated SVD and not to the index of the basis functions).

2. Assignment

For this homework you are asked to perform a MDS on the average rainfull functions for the Canadian cities. In particular:

- choose a set of basis functions (polynomial of Fourier basis with some $m \leq 20$)
- transform the data series for each Canadian city to a fitted function (estimated θ parameteres)
- collect all estimated θ parameters into a $\boldsymbol{\Theta}$ matrix
- perform a MDS on the $\boldsymbol{\Theta}$ matrix
- make an informative graph
- interprete the graph (you can e.g. use the metadata)

You are asked to present your results as an R markdown file. Briefly comment your R code, motivate your choices and provide interpretation of your final results.

There is an R package that contains functions for an FDA. However, you are explicitly asked NOT to use this package. Using the package will not give you deep insight into how an FDA works.