An Introduction to Splines

Trinity River Restoration Program
Workshop on Outmigration: Population Estimation

October 6–8, 2009

1. Linear Regression
   - Simple Regression and the Least Squares Method
   - Least Squares Fitting in `R`
   - Polynomial Regression

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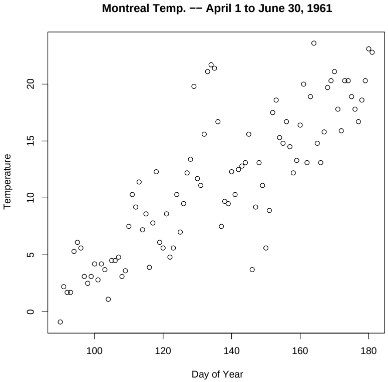
Simple Linear Regression

Daily temperatures in Montreal from April 1 (Day 81) to June 30 (Day 191), 1961.



Assumptions

Mean On average, the change in the response is proportional to the change in the predictor.

Errors
1. The deviation in the response for any observation does not depend on any other observation.
2. The average magnitude of the deviation is the same for all values of the predictor.

Mathematically

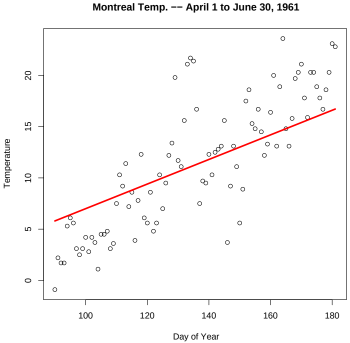
For $i = 1, \ldots, n$:

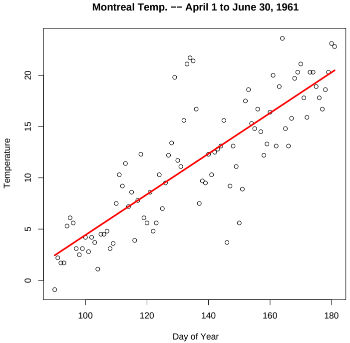
$$y_i = \beta_0 + \beta_1 x_i + \epsilon_i$$

where $\epsilon_1, \ldots, \epsilon_n$ are independent with mean 0 and variance σ^2.

The Least Squares Method

Example: The Montreal Data





Definition

Given values for β_0 and β_1, the residual for the i^{th} observation is the difference between the observed and the predicted response:

$$e_i = y_i - \hat{y}_i$$

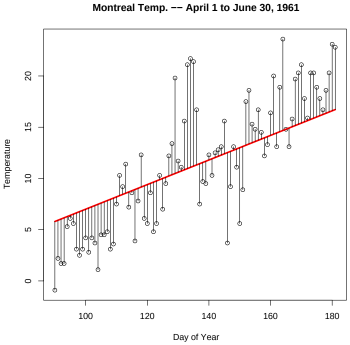
where $\hat{y}_i = \beta_0 + \beta_1 x_i$.

The least squares method defines the best values of β_0 and β_1 to be those that minimize the sum of the squared residuals:

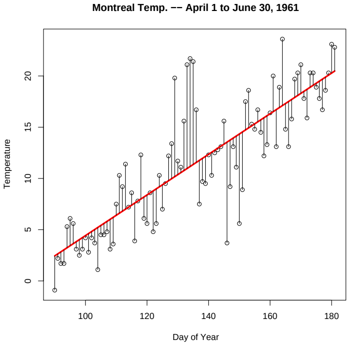
$$SS = \sum_{i=1}^{n} e_i^2 = \sum_{i=1}^{n} (y_i - \hat{y}_i)^2.$$

The Least Squares Method

Example: The Montreal Data



SS=1549.37



SS=1148.56

1. Linear Regression
   - Simple Regression and the Least Squares Method
   - Least Squares Fitting in R
   - Polynomial Regression

Suppose that the data is a data frame with elements:

- x: the days from 90 to 181
- y: the observed temperatures

```
> data = read.table("MontrealTemp1.txt")
> summary(data)
       x                y
 Min.   : 90.0   Min.   :-0.90
 1st Qu.:112.8   1st Qu.: 5.60
 Median :135.5   Median :11.55
 Mean   :135.5   Mean   :11.46
 3rd Qu.:158.2   3rd Qu.:16.70
 Max.   :181.0   Max.   :23.60
>
```

Fitting the model with `lm`:

```
> lm(y~x,data)

Call:
lm(formula = y ~ x, data = data)

Coefficients:
(Intercept)            x
   -15.3996       0.1982
```

Fitting the model with `lm`:

```
> lmfit = lm(y~x,data)
> attributes(lmfit)
$names
 [1] "coefficients"  "residuals"
 [3] "effects"       "rank"
 [5] "fitted.values" "assign"
 [7] "qr"            "df.residual"
 [9] "xlevels"       "call"
[11] "terms"         "model"

$class
[1] "lm"

>
```

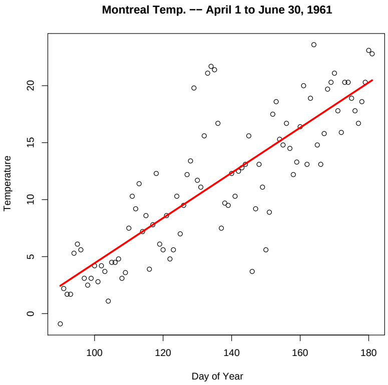
Plotting the fitted line over the raw data:

```
# Plot the raw data
> plot(data$x,data$y,
     main="Montreal Temp. ...",
     xlab="Day of Year",ylab="Temperature")

# Add the fitted line
> lines(data$x,lmfit$fit,col="red",lwd=3)
```

Least Squares Fitting in R

The Fitted Line



Residual Diagnostics

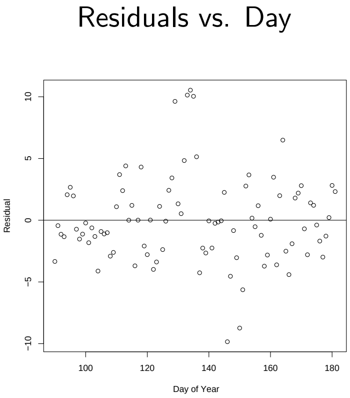
The value of the residuals should not depend on x or y in any systematic way.

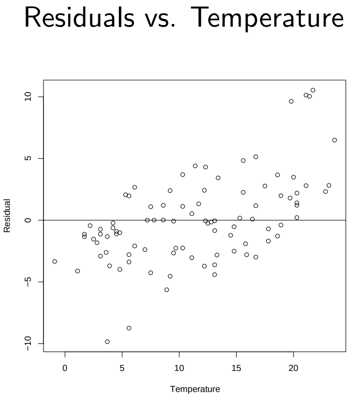
- Common indications of lack of fit:
  - trends with x or y (curves or clusters of high/low values)
  - constant increase/decrease (funnel shape)
  - increase followed by decrease (football shape)
  - very large (+ or -) values (outliers)
- Assessed by plotting e versus x and y.

Plotting the residuals versus the predictor and response:

```
## Plot the residuals versus day
> plot(data$x,lmfit$resid,
       xlab="Day of Year",ylab="Residual")
> abline(h=0)

## Plot the residuals versus temperature
> plot(data$y,lmfit$resid,
       xlab="Temperature",ylab="Residual")
> abline(h=0)
```

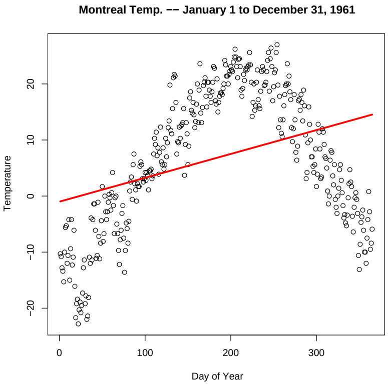

Residuals vs. Day
Residual
10
5
0
−5
−10
100
120
140
160
180
Day of Year


Residuals vs. Temperature
Residual
10
5
0
−5
−10
0
5
10
15
20
Temperature

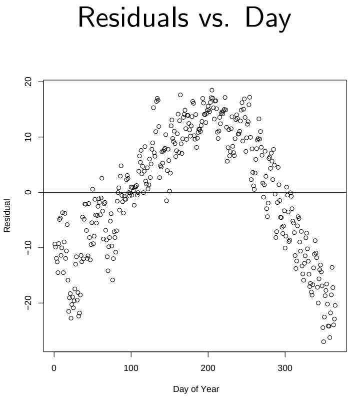
Exercises

1. Montreal Temperature Data – April 1 to June 30, 1961
   File: `Intro_to_splines\Exercises\montreal_temp_1.R`
   Use the provide code to fit the simple linear regression model to the Montreal temperature data from the spring of 1961, plot the fitted line, and produce the residual plots.

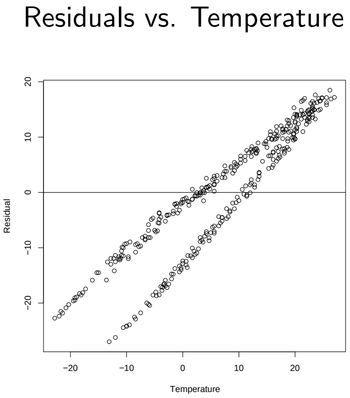
2. Montreal Temperature Data – Jan. 1 to Dec. 31, 1961
   File: `Intro_to_splines\Exercises\montreal_temp_2.R`
   Repeat exercise 1 with the data from all of 1961.



Montreal Temp. -- January 1 to December 31, 1961
Temperature
Day of Year
0
100
200
300
−20
−10
0
10
20



Residuals vs. Day
Residual
Day of Year
20
10
0
−10
−20
0
100
200
300



Residuals vs. Temperature
Residual
Temperature
20
10
0
−10
−20
−20
−10
0
10
20

Definition

A polynomial of degree D is a function formed by linear combinations of the powers of its argument up to D:

$$y = \beta_0 + \beta_1 x + \beta_2 x^2 + \cdots + \beta_D x^D$$

Specific Polynomials

$$\begin{aligned}
\text{Linear} \quad & y = \beta_0 + \beta_1 x \\
\text{Quadratic} \quad & y = \beta_0 + \beta_1 x + \beta_2 x^2 \\
\text{Cubic} \quad & y = \beta_0 + \beta_1 x + \beta_2 x^2 + \beta_3 x^3 \\
\text{Quartic} \quad & y = \beta_0 + \beta_1 x + \beta_2 x^2 + \beta_3 x^3 + \beta_4 x^4 \\
\text{Quintic} \quad & y = \beta_0 + \beta_1 x + \beta_2 x^2 + \beta_3 x^3 + \beta_4 x^4 + \beta_5 x^5
\end{aligned}$$

Definition

The design matrix for a regression model with n observations and p predictors is the matrix with n rows and p columns such that the value of the j^{th} predictor for the i^{th} observation is located in column j of row i.

Design matrix for a polynomial of degree D

$$\begin{array}{c} 1 \\ 2 \\ 3 \\ \vdots \\ n \end{array} \begin{bmatrix} 1 & x_1 & x_1^2 & x_1^3 & \cdots & x_1^D \\ 1 & x_2 & x_2^2 & x_2^3 & \cdots & x_2^D \\ 1 & x_3 & x_3^2 & x_3^3 & \cdots & x_3^D \\ & & & \vdots & & \\ 1 & x_n & x_n^2 & x_n^3 & \cdots & x_n^D \end{bmatrix}$$

The design matrix for polynomial regression can be generated with the function `outer()`:

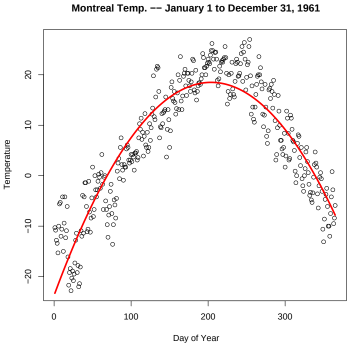
```
> D = 2
> X = outer(data$x,1:D,"^")
> X[1:5,]
     [,1] [,2]
[1,]    1    1
[2,]    2    4
[3,]    3    9
[4,]    4   16
[5,]    5   25
>
```

Note: we do not need to include the intercept column.

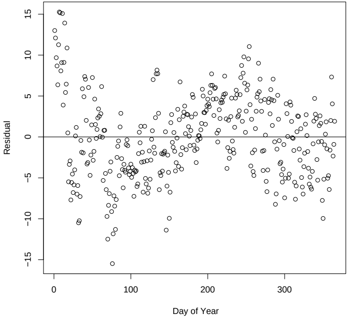
```
> lmfit = lm(y~X,data)
> attributes(lmfit)
$names
 [1] "coefficients"  "residuals" ...

$class
[1] "lm"

> lmfit$coefficients
  (Intercept)             X1            X2
-23.715358962   0.413901580  -0.001014625
```



Montreal Temp. –– January 1 to December 31, 1961
Temperature
Day of Year
-20
-10
0
10
20
0
100
200
300

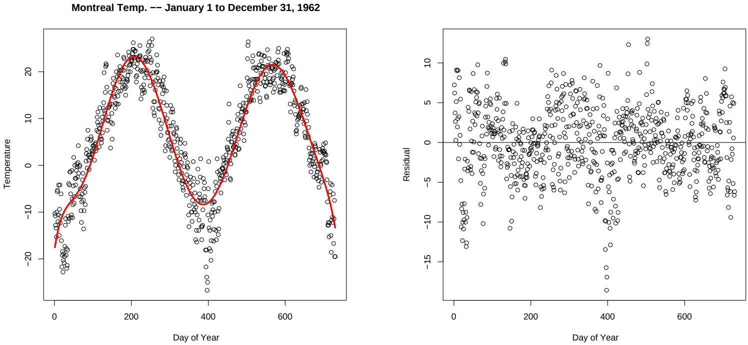


Residual
Day of Year
-15
-10
-5
0
5
10
15
0
100
200
300

EXERCISES

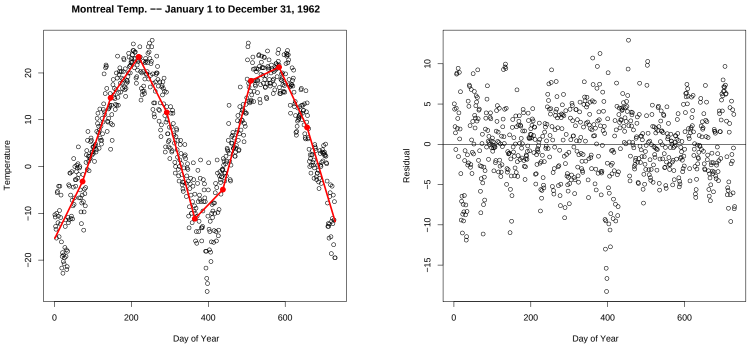
1. Montreal Temperature Data – Jan. 1 to Dec. 31, 1961
   File: `Intro_to_splines\Exercises\montreal_temp_3.R`
   Use the provided code to fit polynomial regression models of varying degree to the data for all of 1961. Models of different degree are constructed by setting the variable `D` (e.g., `D=2` produces a quadratic model). What is the minimal degree required for the model to fit well?

2. Montreal Temperature Data – Jan. 1, 1961, to Dec. 31, 1962
   File: `Intro_to_splines\Exercises\montreal_temp_4.R`
   Repeat this exercise using the data from both 1961 and 1962.



How is the temperature changing in the spring of 1962?

$$y = -7.6 - 8.3x - 0.3x^2 - 5.2 \times 10^4 x^{-3} + 4.4 \times 10^{-6} x^4 \\ - 2.1 \times 10^{-8} x^5 + 6.0 \times 10^{-11} x^6 - 8.9 \times 10^{-14} x^7 + 5.5 \times 10^{-17} x^8$$



How is the temperature changing in the spring of 1962?

$$y = -144.5 + .3x$$

Definition

A linear spline is a continuous function formed by connecting linear segments. The points where the segments connect are called the knots of the spline.

Definition

A spline of degree D is a function formed by connecting polynomial segments of degree D so that:

- the function is continuous,
- the function has $D - 1$ continuous derivatives, and
- the D^{th} derivative is constant between knots.

Definition

The truncated polynomial of degree D associated with a knot ξ_k is the function which is equal to 0 to the left of ξ_k and equal to $(x - \xi_k)^D$ to the right of ξ_k.

$$(x - \xi_k)_+^D = \begin{cases} 0 & x < \xi_k \\ (x - \xi_k)^D & x \geq \xi_k \end{cases}$$

The equation for a spline of degree D with K knots is:

$$y = \beta_0 + \sum_{d=1}^{D} \beta_d x^d + \sum_{k=1}^{K} b_k (x - \xi_k)_+^D$$

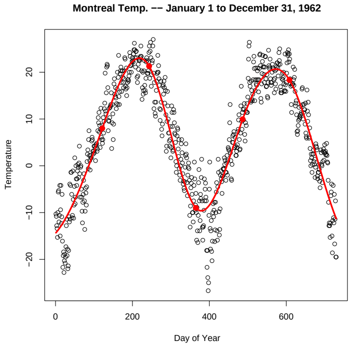
The design matrix for a spline of degree D with K knots is the n by $1 + D + K$ matrix with entries:

$$\begin{bmatrix} 1 & x_1 & x_1^2 & \cdots & x_1^D & (x_1 - \xi_1)_+^D & \cdots & (x_1 - \xi_K)_+^D \\ 1 & x_2 & x_2^2 & \cdots & x_2^D & (x_2 - \xi_1)_+^D & \cdots & (x_2 - \xi_K)_+^D \\ 1 & x_3 & x_3^2 & \cdots & x_3^D & (x_3 - \xi_1)_+^D & \cdots & (x_3 - \xi_K)_+^D \\ & & & \vdots & & & & \\ 1 & x_n & x_n^2 & \cdots & x_n^D & (x_n - \xi_1)_+^D & \cdots & (x_n - \xi_K)_+^D \end{bmatrix}$$

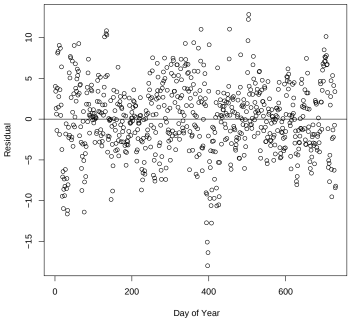
After defining the degree and the locations of the knots, the design matrix can be generated with the functions `outer` and `cbind`:

```
> D = 3
> K = 5
> knots = 730 * (1:K)/(K+1)
> X1 = outer(data$x,1:D,"^")
> X2 = outer(data$x,knots,">") *
       outer(data$x,knots,"-")^D
> X = cbind(X1,X2)
> round(X[c(1,150,300),1:5],1)
     [,1]  [,2]     [,3]      [,4]   [,5]
[1,]    1     1        1       0.0      0
[2,]  150 22500  3375000   22745.4      0
[3,]  300 90000 27000000 5671495.4 181963
>
```

```
lmfit = lm(y~X,data=data)
```



Montreal Temp. –– January 1 to December 31, 1962
Temperature
Day of Year
−20
−10
0
10
20
0
200
400
600



Residual
Day of Year
−15
−10
−5
0
5
10
0
200
400
600

Exercises

1. Montreal Temperature Data – Jan. 1 to Dec. 31, 1961
   File: `Intro_to_splines\Exercises\montreal_temp_5.R`
   Use the code provided to fit splines of varying degree and with different numbers of knots to the data from 1961 and 1962.

Splines computed from the truncated polynomials may be numerically unstable because:

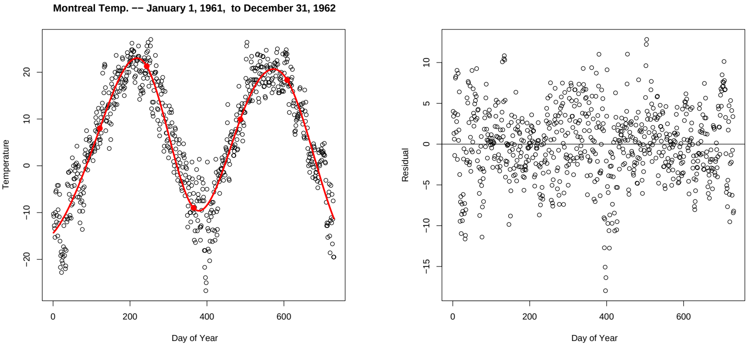
- the values in the design matrix may be very large, and
- the columns of the design matrix may be highly correlated.

The B-spline design matrix can be constructed via the function `bs` provided by the `splines` library:

```
> library(splines)
> D = 3
> K = 5
> knots = 730 * (1:K)/(K+1)
> X = bs(data$x,knots=knots,
         degree=D,intercept=TRUE)
> lmfit = lm(y~X-1,data=data)
>
```

The B-spline Basis in R

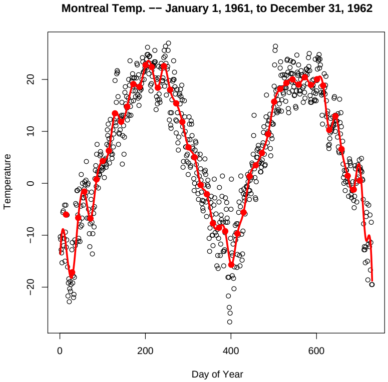
Fitted Cubic B-spline Model



Exercises

1. Montreal Temperature Data – Jan. 1 to Dec. 31, 1961
   File: `Intro_to_splines\Exercises\montreal_temp_6.R`
   Fit B-splines to the data from 1961 and 1962 using the code in the file. Increase the number of knots to see how this affects the fit of the curve. What happens when the number of knots is very large, say $K = 50$?

A cubic spline with 50 knots:



Concept

The shape of a spline can be controlled by carefully choosing the number of knots and their exact locations in order to:

1. allow flexibility where the trend changes quickly, and
2. avoid overfitting where the trend changes little.

Challenge

Choosing the number of knots and their location is a very difficult problem to solve.

Concept

We can also balance overfitting and smoothness by controlling the size of the spline coefficients.

Penalization for the Linear Spline

- Consider the equation for each segment of the spline:

$$
\begin{array}{rcccccc}
(0,\xi_1): & y = & \beta_0 & + & \beta_1 & x \\
(\xi_1,\xi_2): & y = & (\beta_0 - b_1\xi_1) & + & (\beta_1 + b_1) & x \\
(\xi_2,\xi_3): & y = & (\beta_0 - b_1\xi_1 - b_2\xi_2) & + & (\beta_1 + b_1 + b2) & x
\end{array}
$$

- The spline is smooth if $b_1, b_2, \ldots, b_K$ are all close to 0.

Penalized Least Squares

$$PSS = \sum_{i=1}^{n}(y_i - \hat{y}_i)^2 + \lambda \sum_{k=1}^{K} b_k^2$$

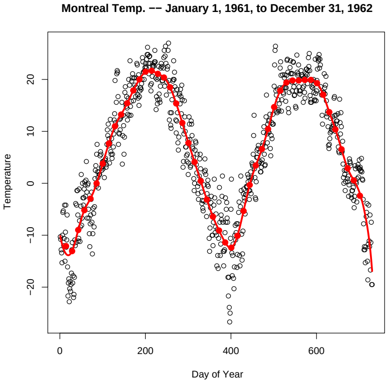
Penalization for the B-spline

The spline is smooth if $b_1, b_2, \ldots, b_K$ are all close to each other.
(But not necessarily close to 0.)

Penalized Least Squares

$$PSS = \sum_{i=1}^{n} (y_i - \hat{y}_i)^2 + \lambda \sum_{k=3}^{K} ((b_k - b_{k-1}) - (b_{k-1} - b_{k-2}))^2$$

A penalized cubic B-spline with 50 knots and $\lambda = 5$:



1. Montreal Temperature Data – Jan. 1 to Dec. 31, 1961
   File: `Intro_to_splines\Exercises\montreal_temp_7.R`
   Fit penalized cubic B-splines to the Montreal temperature data for 1961 and 1962 using the provided code.