An Introduction to Splines

Trinity River Restoration Program
Workshop on Outmigration: Population Estimation

October 6–8, 2009

An Introduction to Splines

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

2. Smoothing Splines
   - Simple Splines
   - B-splines
   - Overfitting and Smoothness

An Introduction to Bayesian Inference

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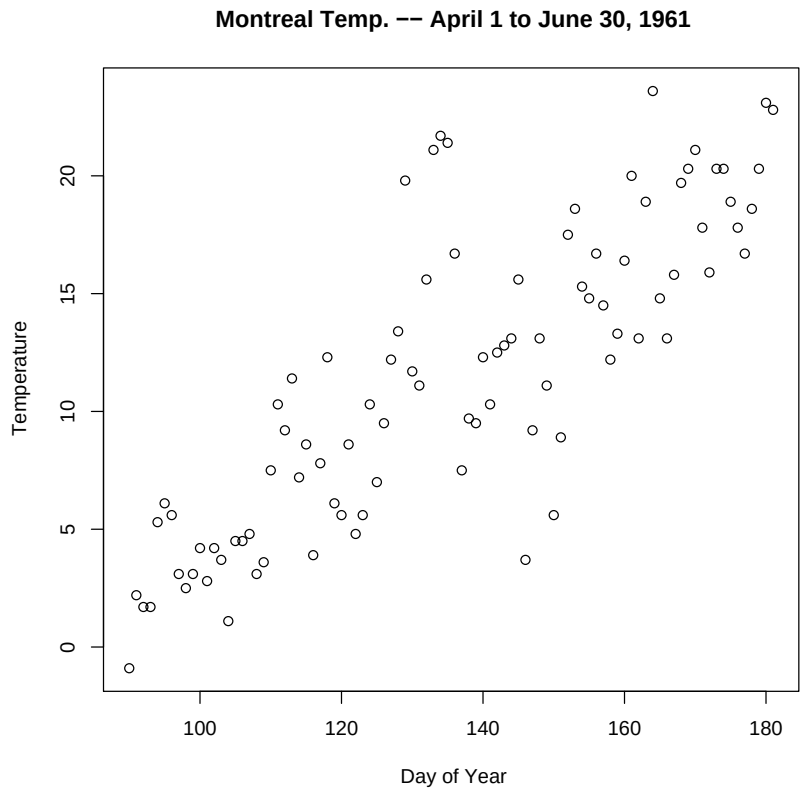
Simple Linear Regression

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

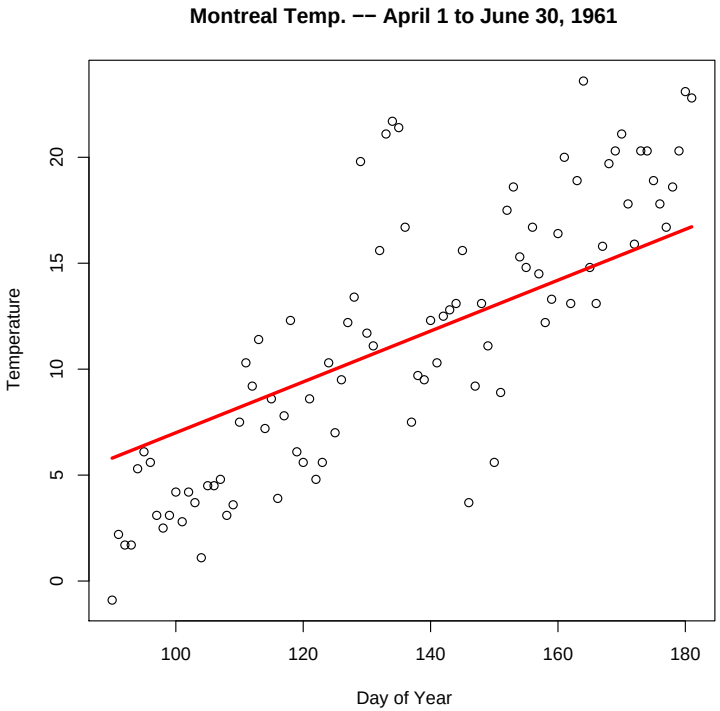
For $i = 1, \ldots, n$:

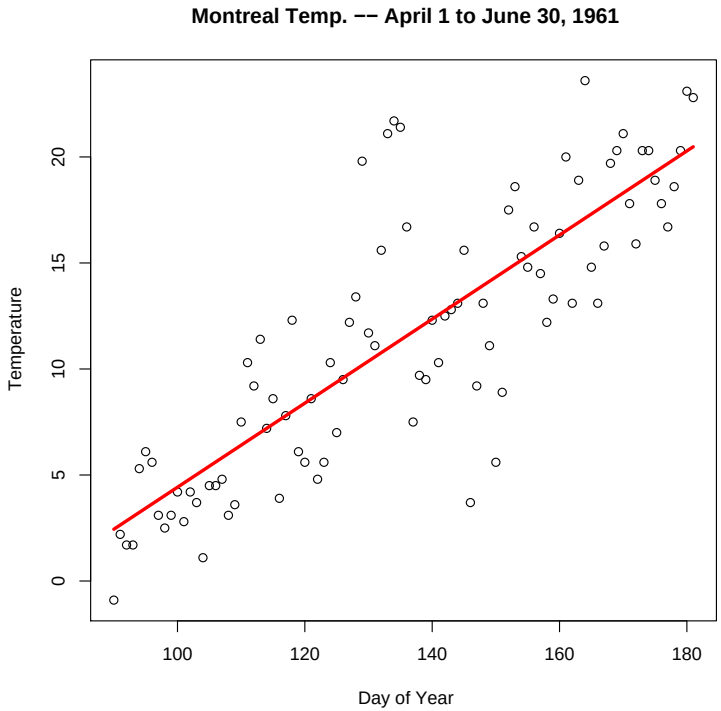
$$y_i = \beta_0 + \beta_1 x_i + \epsilon_i$$

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:

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

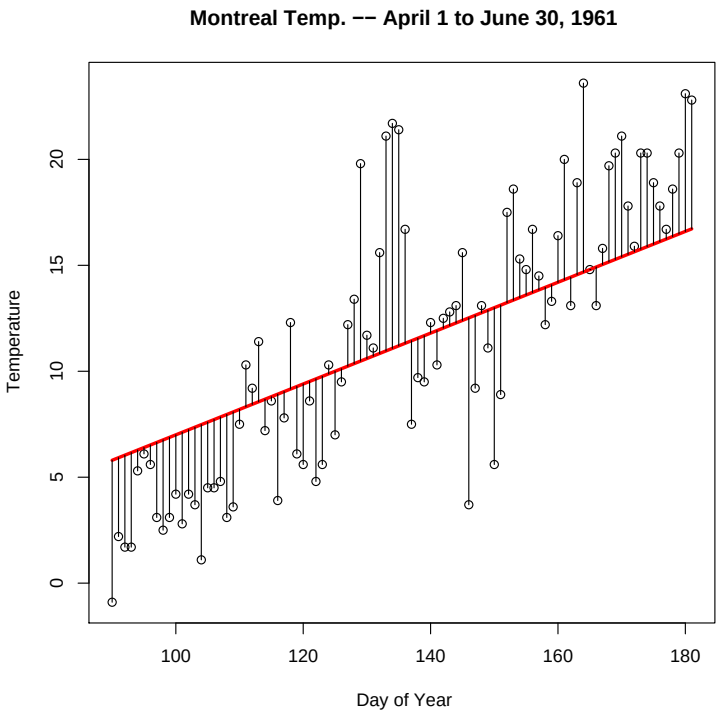
where $\hat{y}_i = \beta_0 + \beta_1 x_i$.

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:

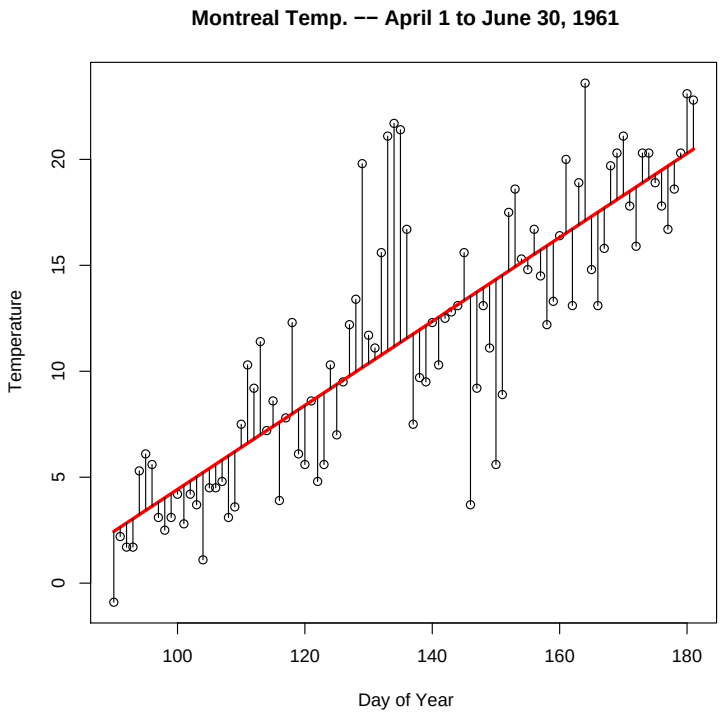
$$SS = \sum_{i=1}^{n} e_i^2 = \sum_{i=1}^{n} (y_i - \hat{y}_i)^2.$$

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

Least Squares Fitting in R

The Data

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"

>
```

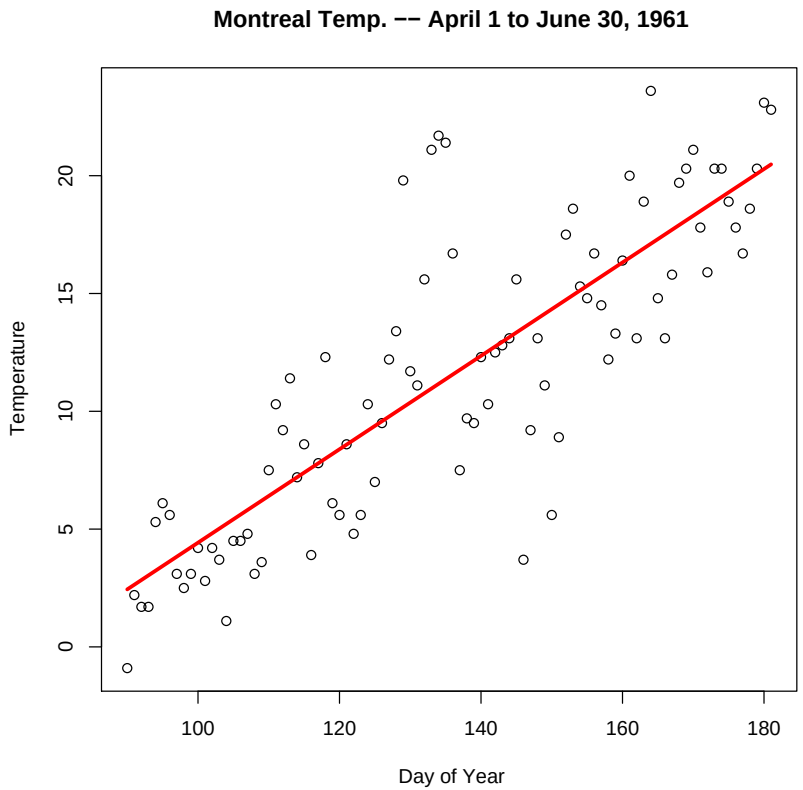
Plotting the fitted line over the raw data:

```
# 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.

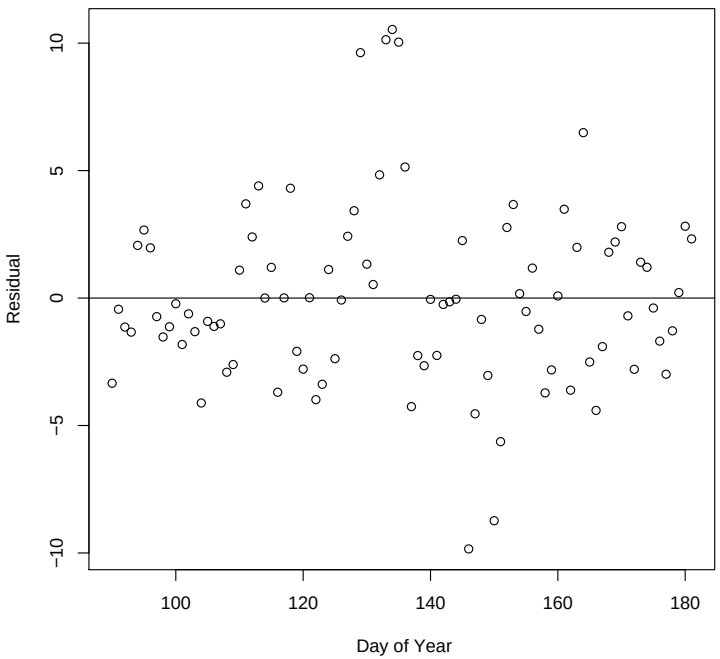
- Common indications of lack of fit:
  - trends with x or y (curves or clusters of high/low values)
  - constant increase/decrease (funnel shape)
  - increase followed by decrease (football shape)
  - very large (+ or -) values (outliers)
- Assessed by plotting e versus x and y.

Plotting the residuals versus the predictor and response:

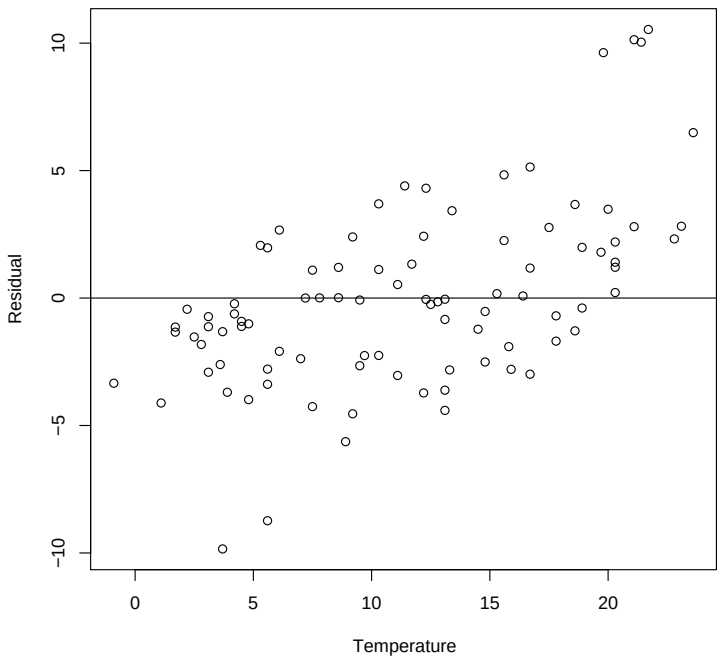
```
## Plot the residuals versus day
> plot(data$x,lmfit$resid,
       xlab="Day of Year",ylab="Residual")
> abline(h=0)

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

Residuals vs. Day



Residuals vs. 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.

1. Linear Regression
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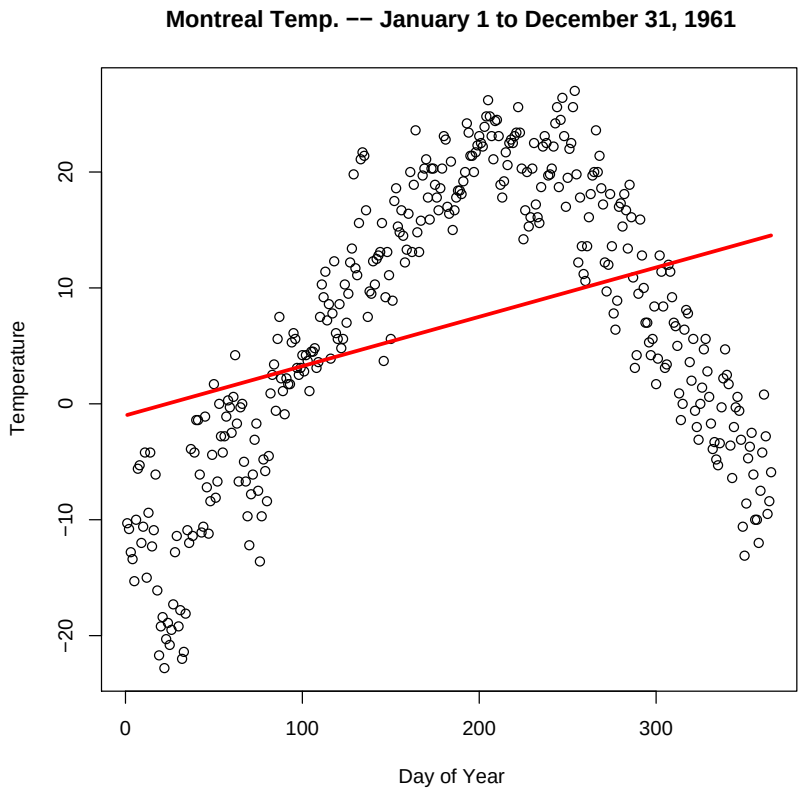
   - Polynomial Regression

Polynomial Regression

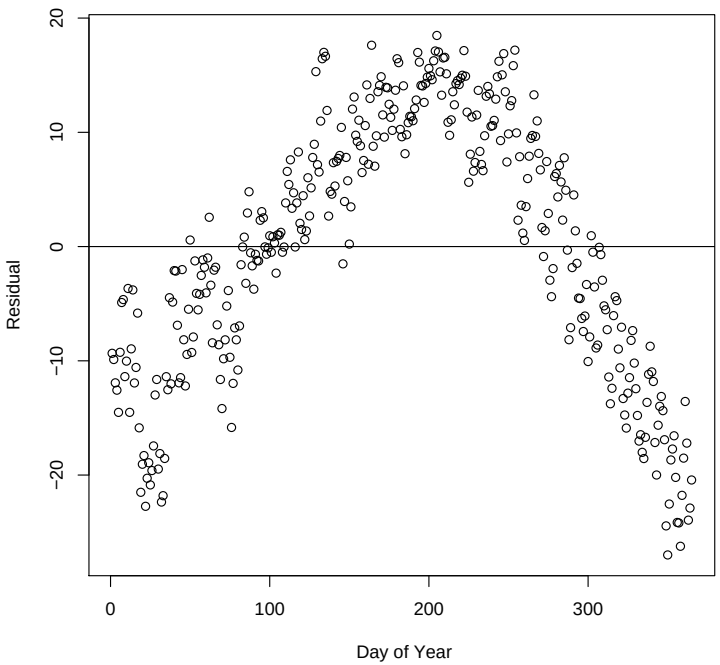
Motivation



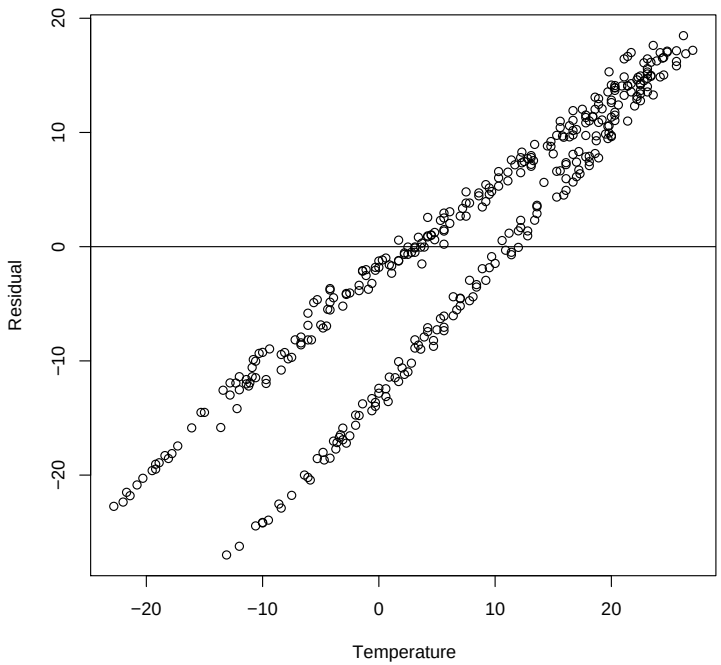
Polynomial Regression

Motivation

Residuals vs. Day



Residuals vs. Temperature



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

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

Polynomial Regression in R

Constructing the Design Matrix – Quadratic

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.

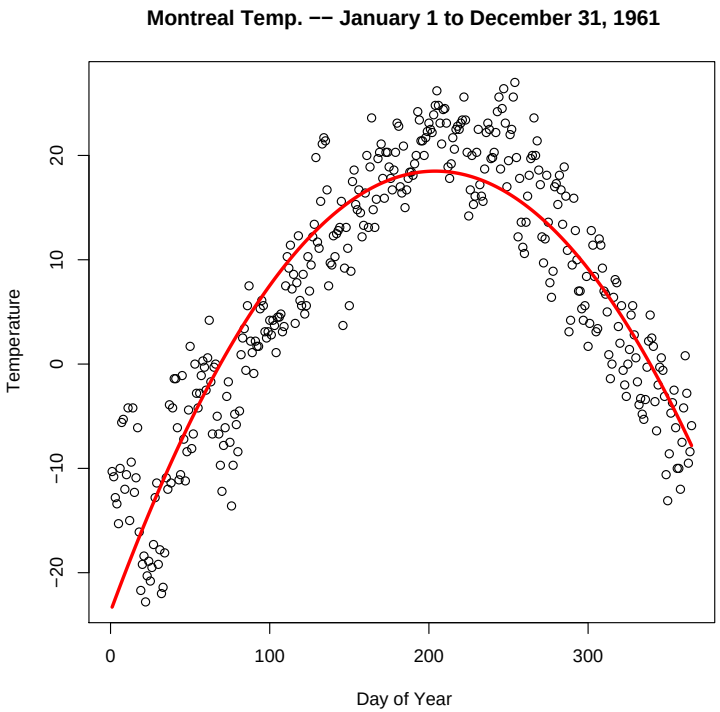
Polynomial Regression in R

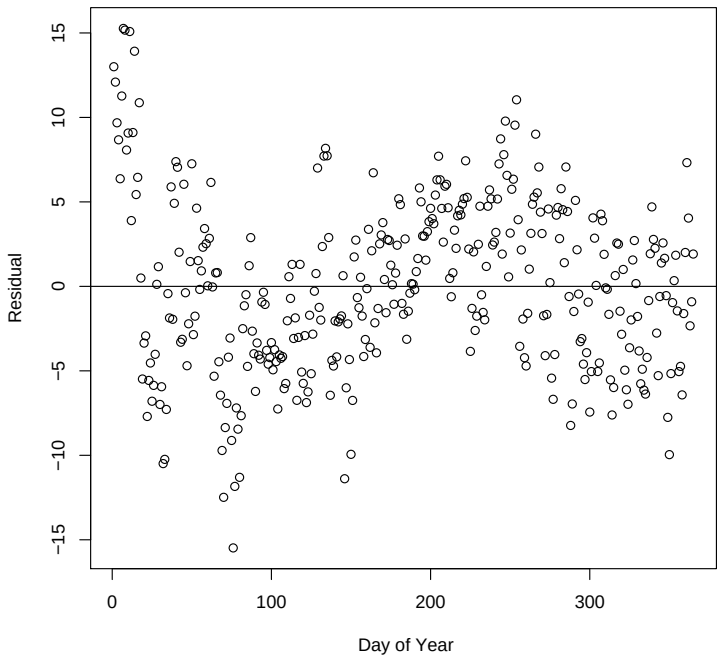
Least Squares Fitting – Quadratic

```
> 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
```

Polynomial Regression in R

Fitted Model – Quadratic





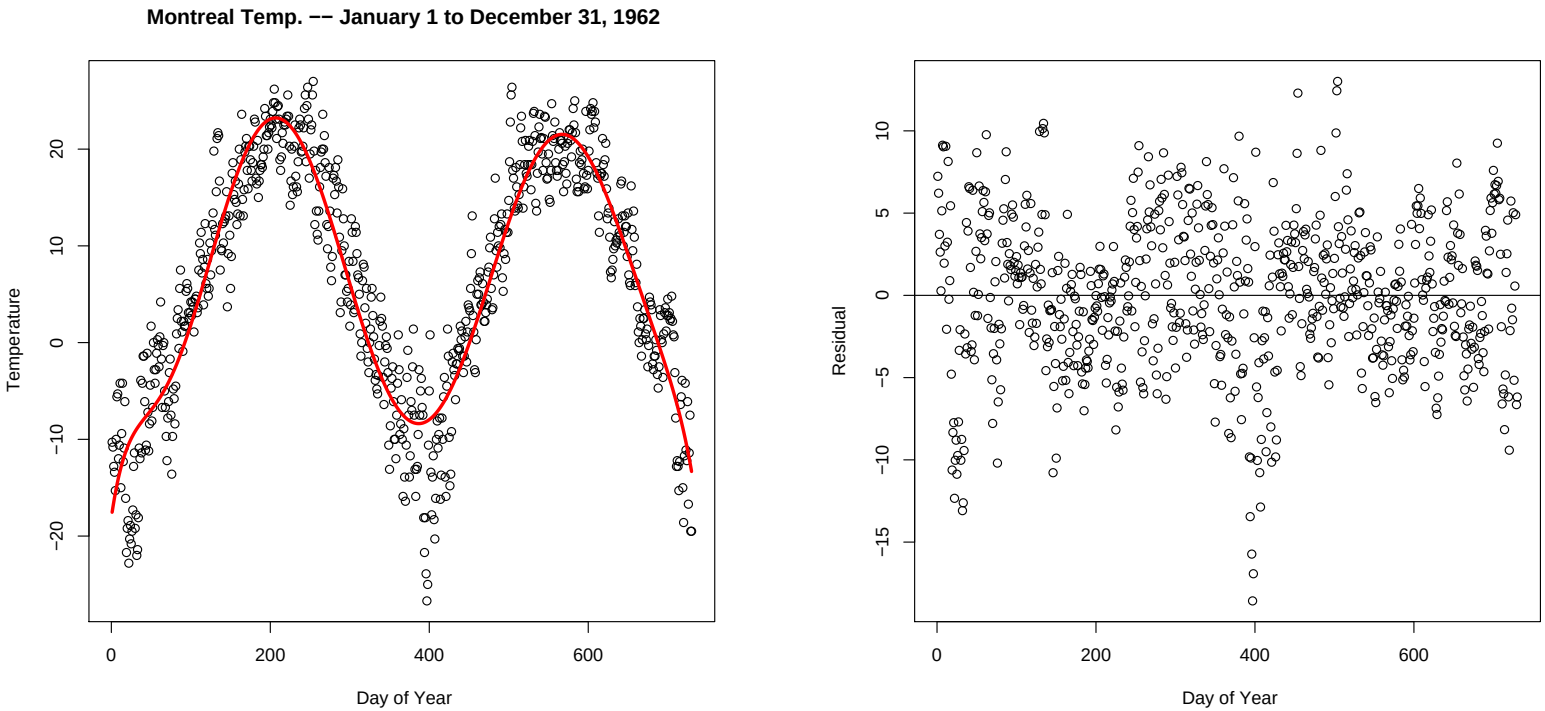
Exercises

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.

2. Smoothing Splines
   - Simple Splines
   - B-splines
   - Overfitting and Smoothness

2 Smoothing Splines
- Simple Splines
- B-splines
- Overfitting and Smoothness

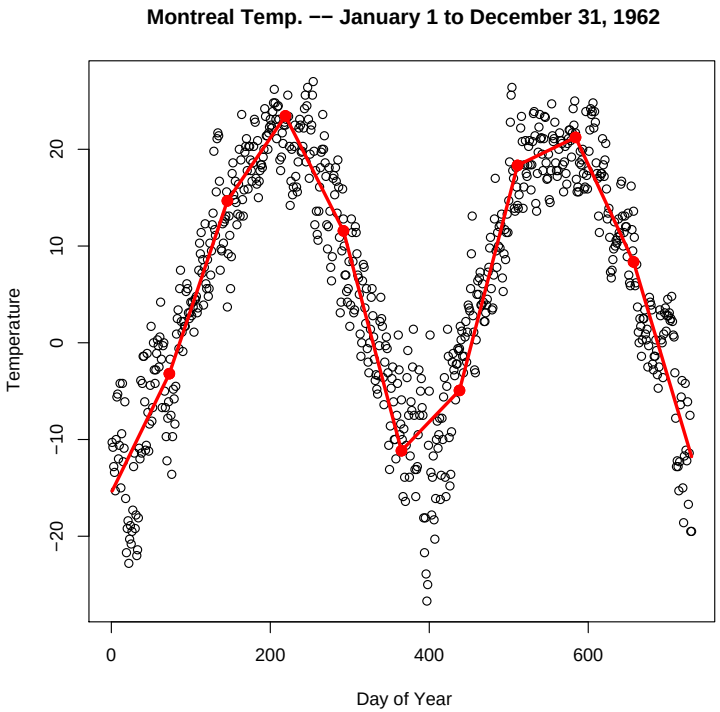


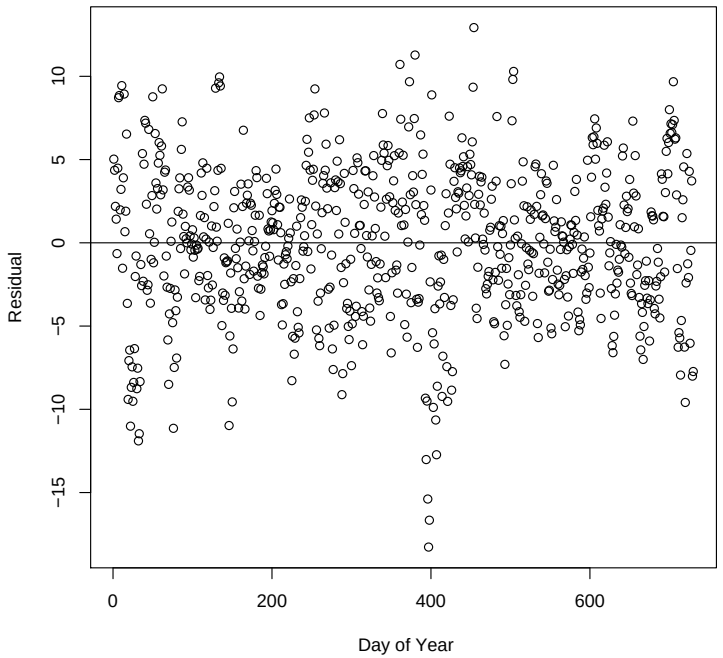
How is the temperature changing in the spring of 1962?

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

Splines

A Linear Spline for the Montreal Temperature Data





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:

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

Simple Splines in R

The Design Matrix

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
>
```

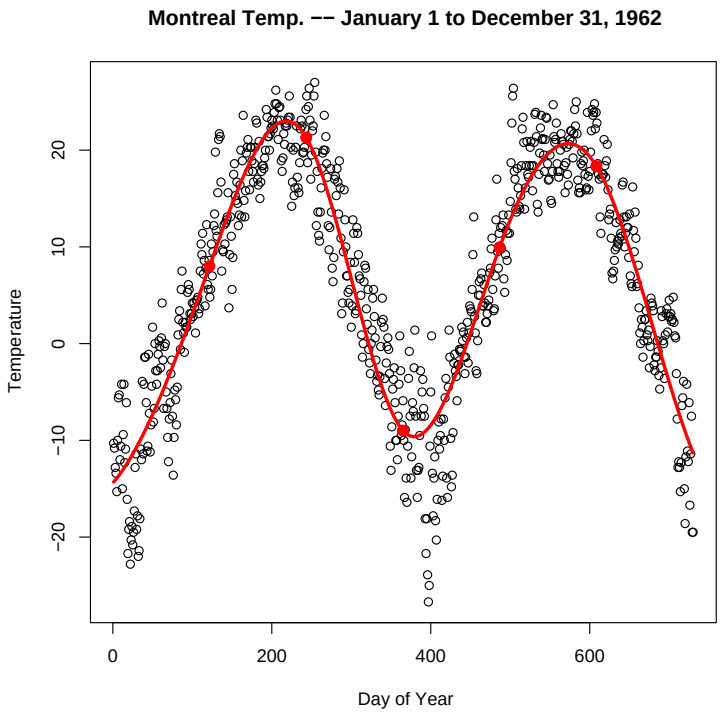
Simple Splines in R

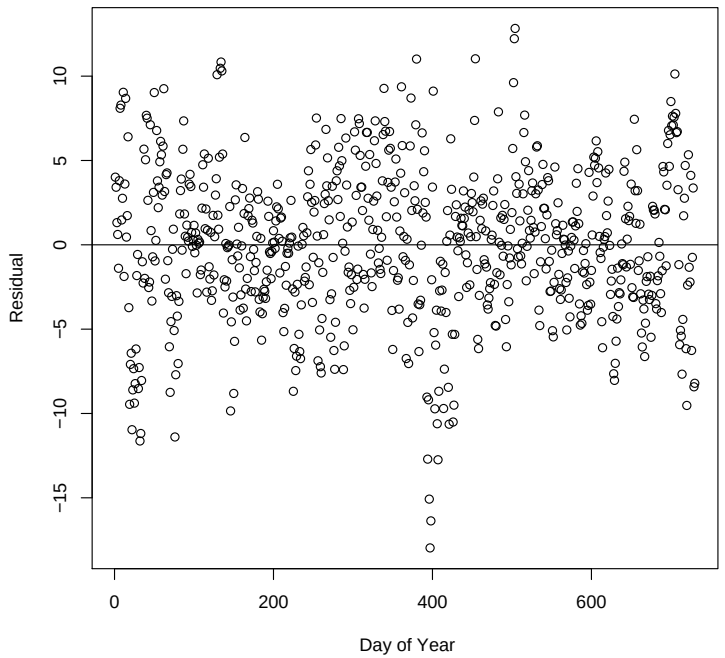
Fitting the Spline Model

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

Simple Splines in R

Fitted Cubic Spline





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.

2 Smoothing Splines
- Simple Splines
- B-splines
- Overfitting and Smoothness

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 Basis in R

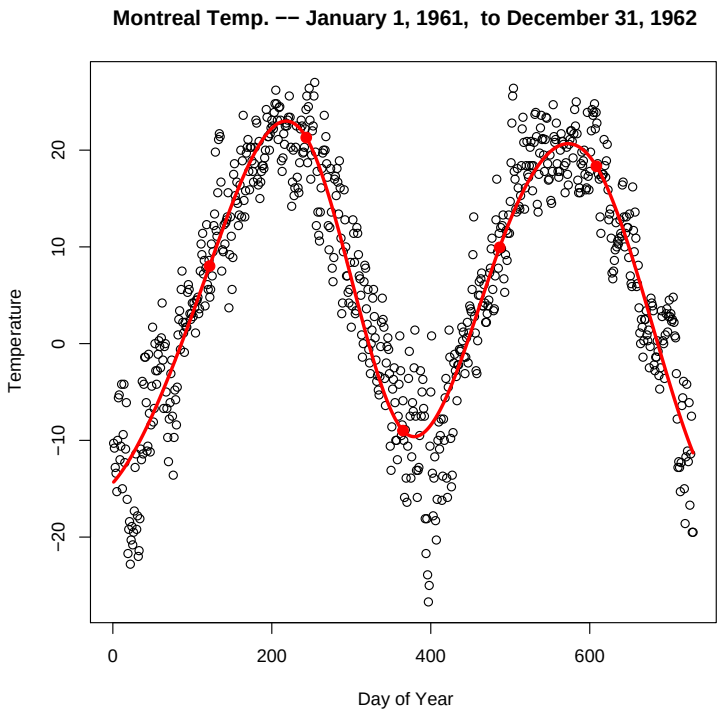
Generating the Design Matrix and Fitting the Model

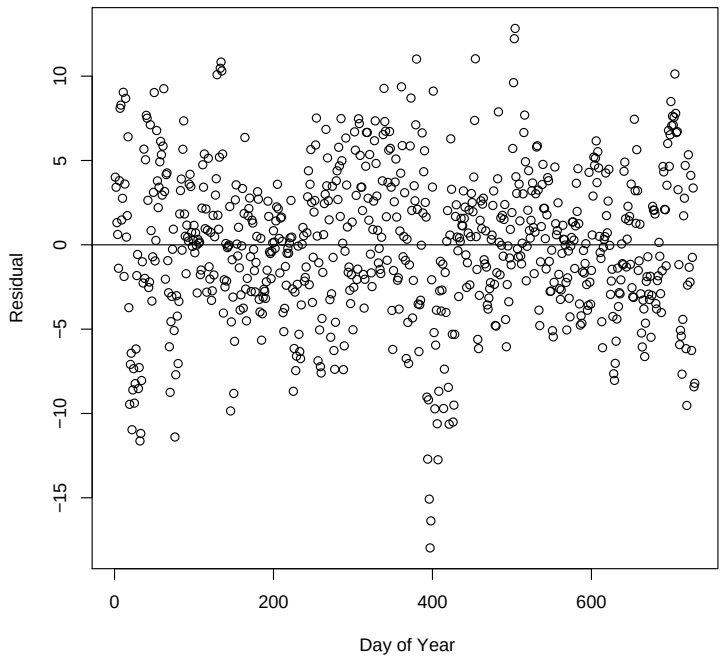
The B-spline design matrix can be constructed via the function `bs` provided by the `splines` library:

```
> 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 $K = 50$?

2 Smoothing Splines
- Simple Splines
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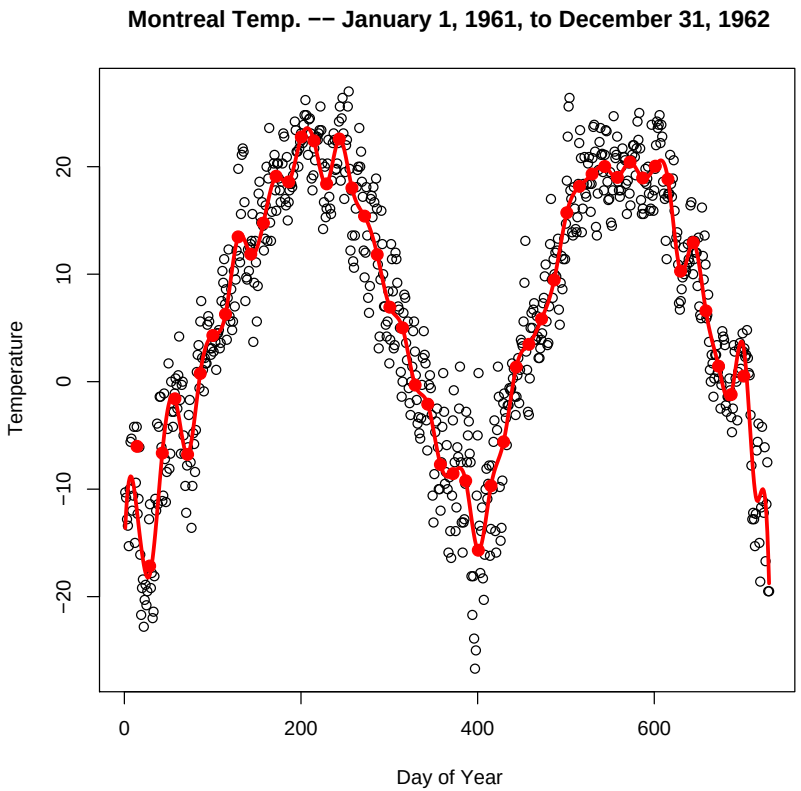
A cubic spline with 50 knots:



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:

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

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

Penalized Least Squares

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

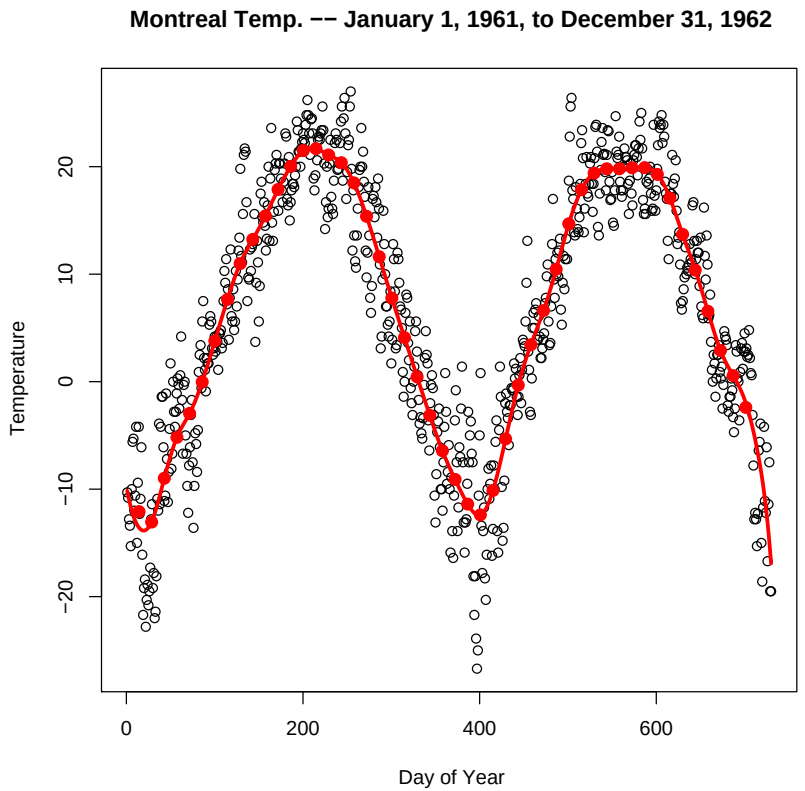
Penalization for the B-spline

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 $\lambda = 5$:



Exercises

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.