M7777 Applied Functional Data Analysis

3. From Data to Functions – Smoothing

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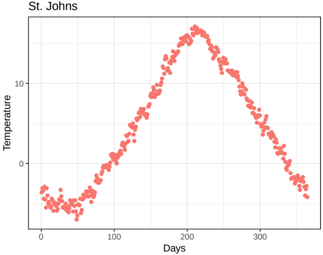
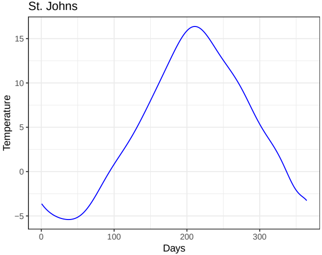
From Data to Functions

How do we go from

data to functions?





Basis Expansions

We consider

$$y_i = x(t_i) + \varepsilon_i, \qquad \varepsilon_i \sim i.i.d$$

and

$$x(t_i) = \sum_{j=1}^{K} c_j \Phi_j(t_i). \tag{1}$$

Let us denote

- $\mathbf{y} = (y_1, \ldots, y_N)'$, $\mathbf{x} = (x(t_1), \ldots, x(t_N))'$
- $\mathbf{\Phi}$ . . . a $N \times K$ matrix containing values $\Phi_j(t_i)$
- $\mathbf{c} = (c_1, \ldots, c_K)'$ . . . **basis coefficients**

We can write (1) as

$$\mathbf{x} = \mathbf{\Phi}\mathbf{c}.$$

Least Squares

How to find $\mathbf{c}$?
Minimize the sum of squared errors

$$SSE(\mathbf{c}) = \sum_{i=1}^{N} (y_i - x(t_i))^2 = (\mathbf{y} - \mathbf{\Phi c})'(\mathbf{y} - \mathbf{\Phi c})$$

This is just linear regression!
The SSE is minimized by the **ordinary least squares** estimate

$$\hat{\mathbf{c}} = \left(\mathbf{\Phi}'\mathbf{\Phi}\right)^{-1} \mathbf{\Phi}'\mathbf{y}.$$

Thus we have the estimate

$$\hat{\mathbf{x}}(t) = \mathbf{\Phi}^*(t) \left(\mathbf{\Phi}'\mathbf{\Phi}\right)^{-1} \mathbf{\Phi}'\mathbf{y}.$$

Standard model: suppose i.i.d $\varepsilon_i \Rightarrow E(\mathbf{y}) = \mathbf{\Phi c}$, $\mathrm{Var}(\mathbf{y}) = \sigma^2 \mathbf{I}_N$

Weighted Least Squares

Practical problems

- heteroscedastic data
- autocorrelated data

Partial solution: **Weighted** Least Squares

$$WSSE(\mathbf{c}) = \sum_{i=1}^{N} w_i^2 (y_i - x(t_i))^2 = (\mathbf{y} - \mathbf{\Phi c})' \mathbf{W}' \mathbf{W} (\mathbf{y} - \mathbf{\Phi c})$$

with $\mathbf{W} = diag\{w_1, \ldots, w_N\}$.
We get an estimate

$$\hat{\mathbf{x}}(t) = \mathbf{\Phi}^*(t) \left(\mathbf{\Phi}' \mathbf{W} \mathbf{\Phi} \right)^{-1} \mathbf{\Phi}' \mathbf{W} \mathbf{y}.$$

and fitted values

$$\hat{\mathbf{y}} = \mathbf{\Phi} \left(\mathbf{\Phi}' \mathbf{W} \mathbf{\Phi} \right)^{-1} \mathbf{\Phi}' \mathbf{W} \mathbf{y} = \mathbf{S} \mathbf{y}.$$

S ... **smoothing matrix**.

Choosing the Number of Basis Functions

How many basis functions?

- Small numbers of basis functions mean little flexibility.
- Larger numbers of basis functions add flexibility, but may "overfit".
- For Monomial and Fourier bases, just add functions to the collection.
- Spline bases: adding knots or increasing the order changes the basis.

Trade off:

- Too many basis functions over-fits the data and reflect errors of measurement.
- Too few basis functions fails to capture interesting features of the curves.

Bias and Variance Tradeoff

Measure of quality of $\hat{x}(t)$

- **Bias**

$$Bias[\hat{x}(t)] = E[\hat{x}(t)] - x(t)$$

- **Variance**

$$\mathrm{Var}[\hat{x}(t)] = E\left\{\hat{x}(t) - E[\hat{x}(t)]\right\}^2$$

- Too many basis functions $\Rightarrow$ small bias, large sampling variance.
- Too few basis functions $\Rightarrow$ small sampling variance, large bias.
- **M**ean **S**quared **E**rror

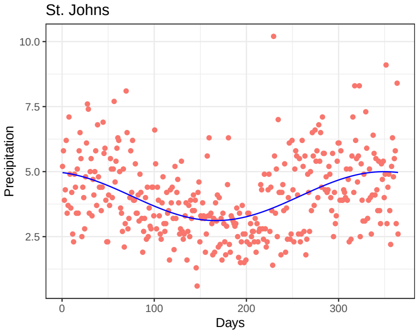
$$MSE[\hat{x}(t)] = E\left[\{\hat{x}(t) - x(t)\}^2\right] = Bias^2[\hat{x}(t)] + \mathrm{Var}[\hat{x}(t)]$$

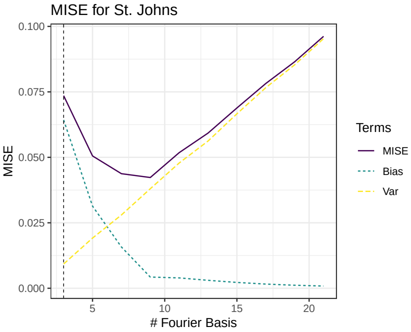
- **I**ntegrated **M**ean **S**quared **E**rror

$$IMSE[\hat{x}(t)] = \int MSE[\hat{x}(t)]dt$$

Choosing the Number of Basis Functions

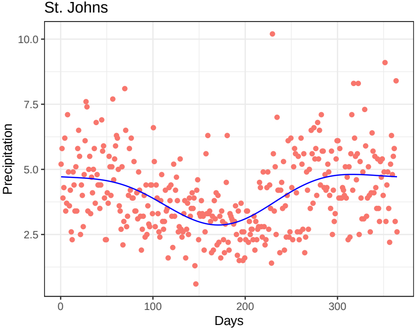
St. Johns Precipitation: **3** Fourier Bases

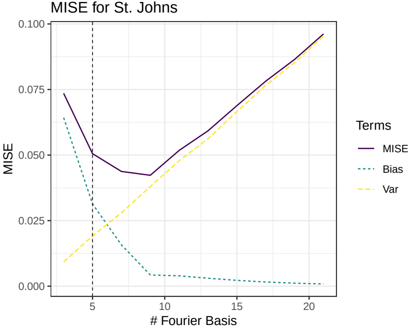




Choosing the Number of Basis Functions

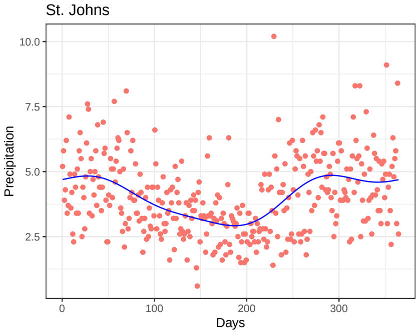
St. Johns Precipitation: **5** Fourier Bases

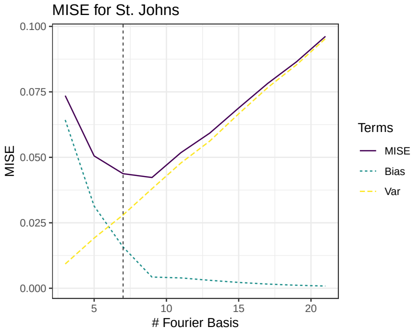




Choosing the Number of Basis Functions

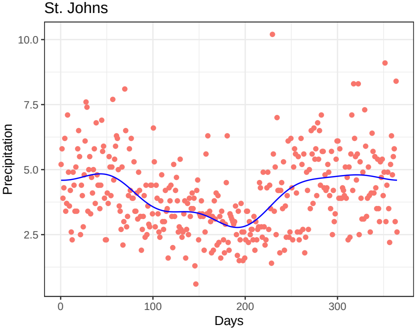
St. Johns Precipitation: **7** Fourier Bases

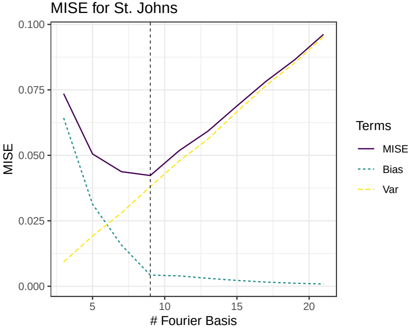




Choosing the Number of Basis Functions

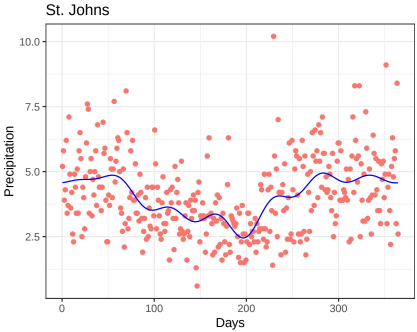
St. Johns Precipitation: **9** Fourier Bases

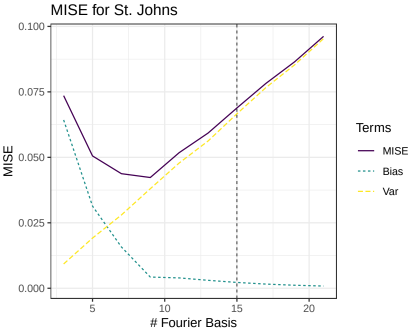




Choosing the Number of Basis Functions

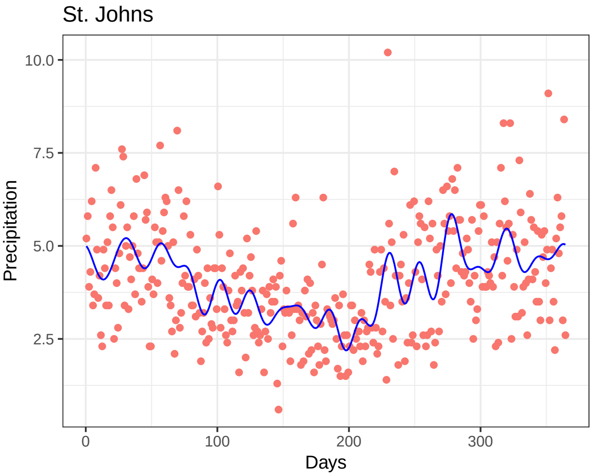
St. Johns Precipitation: **15** Fourier Bases





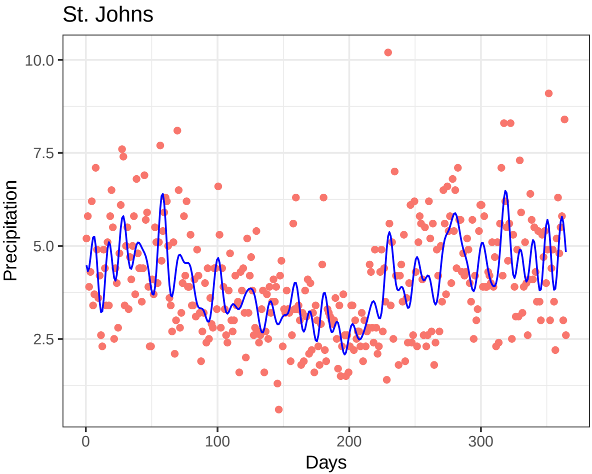
Choosing the Number of Basis Functions

St. Johns Precipitation: **35** Fourier Bases



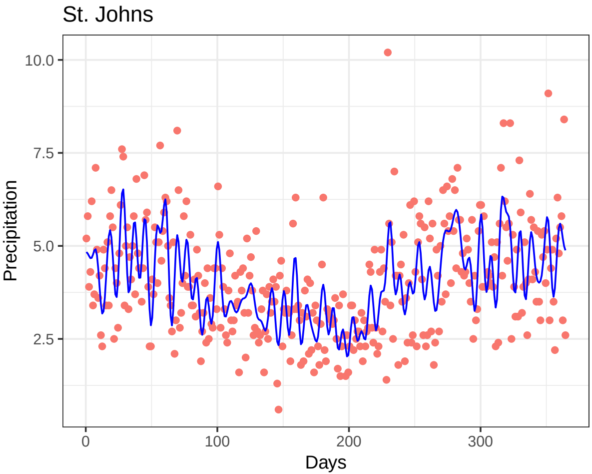
Choosing the Number of Basis Functions

St. Johns Precipitation: **75** Fourier Bases



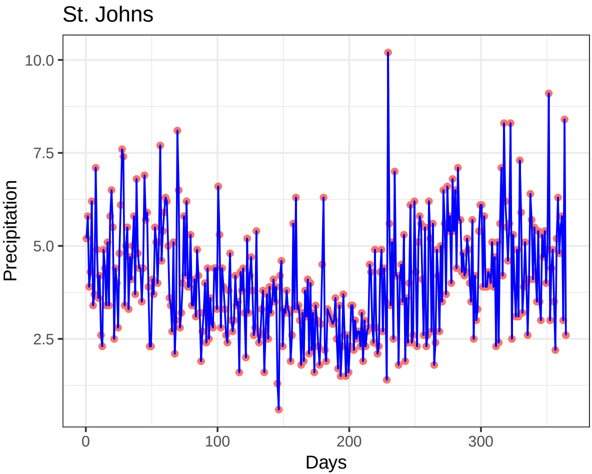
Choosing the Number of Basis Functions

St. Johns Precipitation: **105** Fourier Bases



Choosing the Number of Basis Functions

St. Johns Precipitation: **365** Fourier Bases



Choosing the Number of Basis Functions

Cross-Validation

- Leave out one observation (t_i, y_i) and construct an estimate $\hat{x}_{-i}(t)$ from remaining data.
- Choose K to minimize the **ordinary cross-validation** score

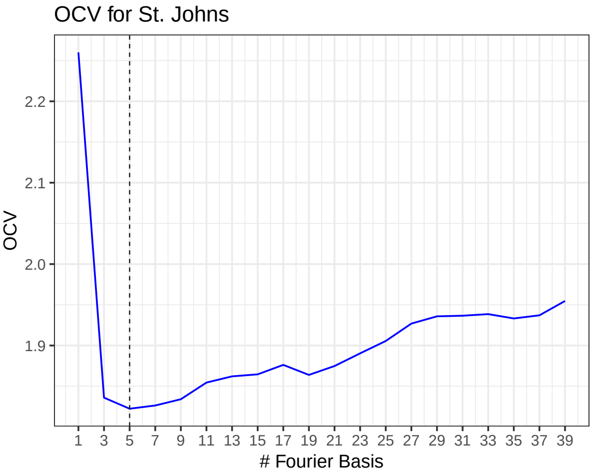
$$OCV(\hat{x}) = \frac{1}{N} \sum_{i=1}^{N} \left(y_i - \hat{x}_{-i}(t_i)\right)^2 .$$

- For a linear smooth $\hat{\mathbf{y}} = \mathbf{S}\mathbf{y}$

$$OCV(\hat{x}) = \frac{1}{N} \sum_{i=1}^{N} \frac{\left(y_i - \hat{x}(t_i)\right)^2}{(1 - s_{ii})^2}.$$

Choosing the Number of Basis Functions

St. Johns Precipitation: Cross-Validated Error



Pointwise Confidence Bands

Estimating the Variance

- Standard model assumes

$$\mathrm{Var}[\mathbf{y}] = \sigma^2 \mathbf{I}_N$$

- An unbiased estimate (can be more sophisticated for correlated residuals)

$$\hat{\sigma}^2 = \frac{1}{N-K} SSE(\hat{\mathbf{c}})$$

- For a linear smooth $\hat{\mathbf{y}} = \mathbf{S}\mathbf{y}$

$$\mathrm{Var}[\hat{\mathbf{y}}] = \sigma^2 \mathbf{S}\mathbf{S}'.$$

- More generally, for $\mathrm{Var}[\mathbf{y}] = \mathbf{\Sigma}$

$$\mathrm{Var}[\hat{\mathbf{y}}] = \mathbf{S}\mathbf{\Sigma}\mathbf{S}'.$$

Pointwise Confidence Bands

Pointwise Confidence Intervals

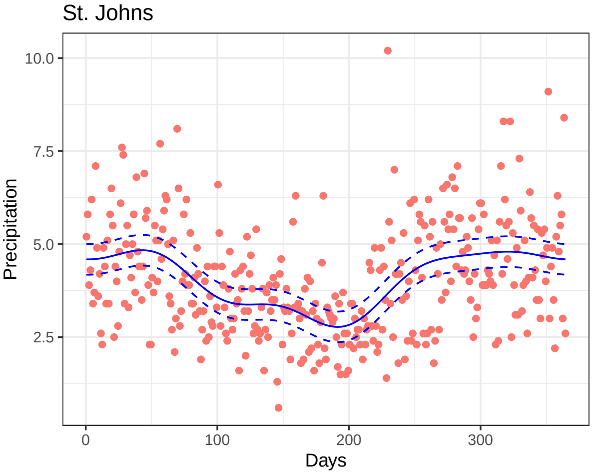
- For each point we calculate lower and upper bands for $\hat{\mathbf{y}}$ by

$$\hat{\mathbf{y}} \pm u_{0.975}\sqrt{\mathrm{Var}[\hat{\mathbf{y}}]}.$$

- These bands are not confidence bands for the entire curve, but only for the value of the curve at a fixed point.
- Ignores bias in the estimated curve.
- Provide an impression of how well the curve is estimated.

Choosing the Number of Basis Functions

Fitted St. Johnes Precipitation Data with 9 Fourier Bases and Confident Bands



Problems to solve

1. Melanoma Data
   - Load the variable `melanoma` from the `fda` package and plot it.
   - Fit these data with a Fourier basis, choosing the number of basis functions by minimizing the gcv value returned by smooth.basis. Plot the Cross-Validation function and the final fit (see Figures 1,2).
   - Try removing a linear trend for these data first, by looking at the residuals after a call to lm. Repeat the steps above; does the optimal number of basis functions change?
   - Re-fit the data using an gcv-optimal B-spline basis. Plot the CV function for this basis and the final fit (see Figures 3,4).
   - Plot the previous fit with its pointwise 95% confidence bands (see Figure 5). What's the observed value of incidences in 1950? What's the estimated mean confidence band for this year?

     [2.2, $(2.49, 2.96)$]

Problems to solve

2. Canadian Weather Data
   - Load the variable `CanadianWeather` from the `fdа` package and select the precipitation in St. Johns.
   - Fit these data using a B-spline basis with 5 basis functions.
   - What's the observed value of precipitation in St. Johns on January 23? What's the estimated mean confidence band for this day?

     $[4.4,\ (4.37, 4.98)]$

Problems to solve

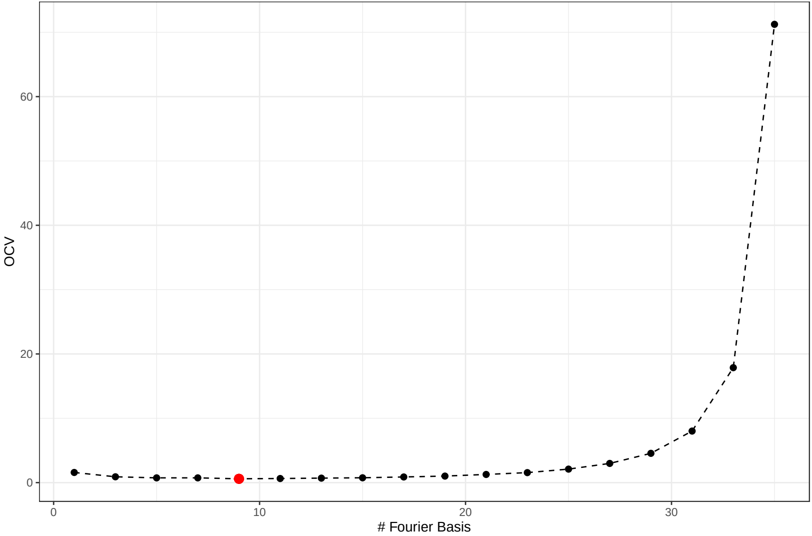


Figure 1.

Problems to solve

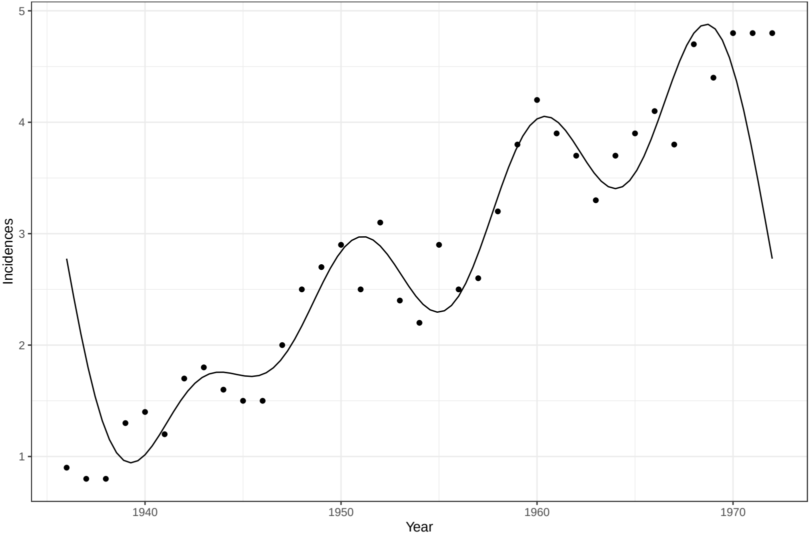


Figure 2.

Problems to solve

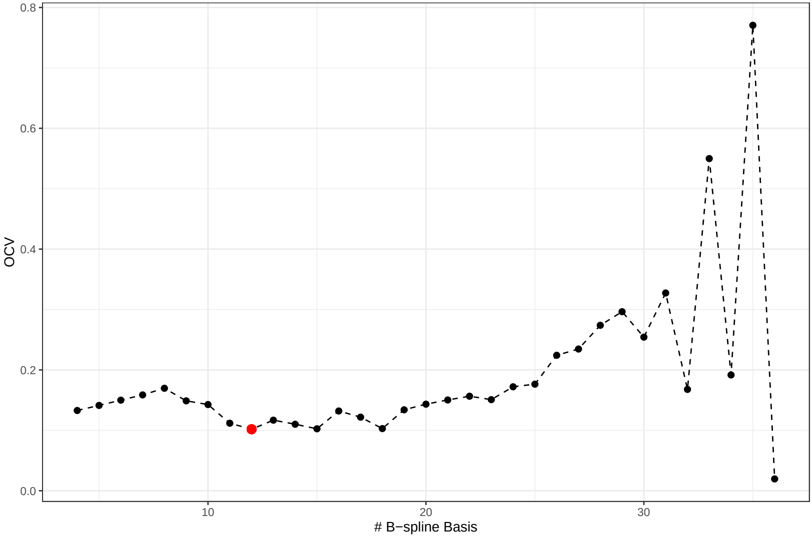


Figure 3.

Problems to solve

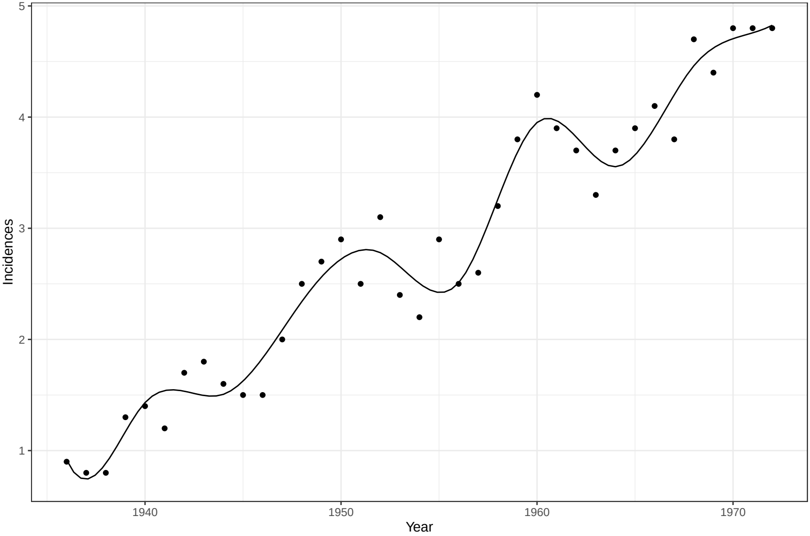


Figure 4.

Problems to solve

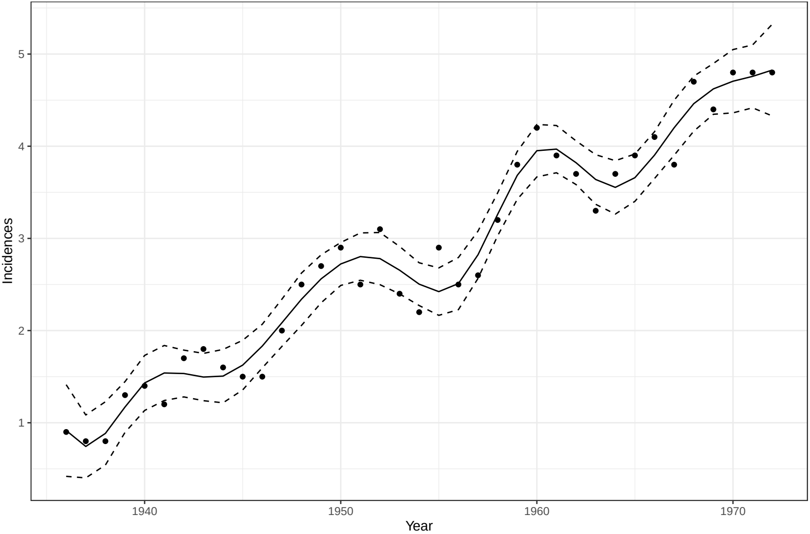


Figure 5.