STAT406- Methods of Statistical Learning
Lecture 8

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UBC - Sep / Dec 2017

POLICE DATA CHALLENGE

Help Make Communities Safer Using Statistics

The American Statistical Association and the Police Data Initiative are calling on high school and college undergraduate students to compete in the Police Data Challenge.

Explore public data sets on calls for police service in Baltimore, Cincinnati, and Seattle. Make recommendations for innovative solutions to enhance public safety.

- A $50 Amazon gift card
- Bragging rights
- The chance to have an impact on local communities

Complete online intent form by **October 6, 2017**

Entries due **November 3, 2017**

For contest details, visit
thisisstatistics.org/policedatachallenge

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@ThisIsStats

More flexible regression

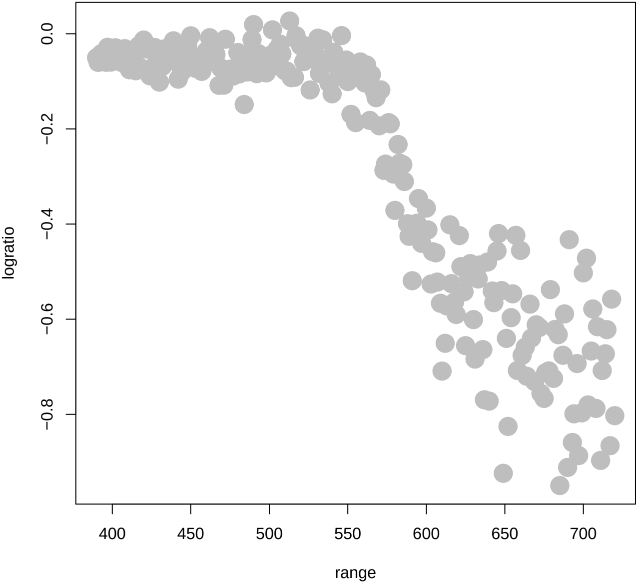
- What if the regression function

$$E\left[Y|\mathbf{X}\right] = f\left(\mathbf{X}\right)$$

  is not linear?

- Example LIDAR

LIDAR



Non-linear regression

- Model: $E\left[Y | X_1, X_2, \ldots, X_p\right] = f\left(X_1, X_2, \ldots, X_p; \theta_1, \theta_2, \ldots, \theta_k\right)$
- This is typically a non-linear model
- But it is fully parametric
- The parameters are $\theta_1, \theta_2, \ldots, \theta_k$
- Using MLE (or LS) we can obtain estimates $\hat{\theta}_1$, ..., $\hat{\theta}_k$
- ... and associated standard errors!

Non-linear regression

- Sometimes it's difficult to find an appropriate family of functions

- Polynomials are a natural choice

$$m(x) = m(x_0) + \frac{1}{2} m'(x_0)(x - x_0) + \cdots$$

$$+ \frac{1}{k!} m^{(k-1)}(x_0)(x - x_0)^{k-1} + R_k$$

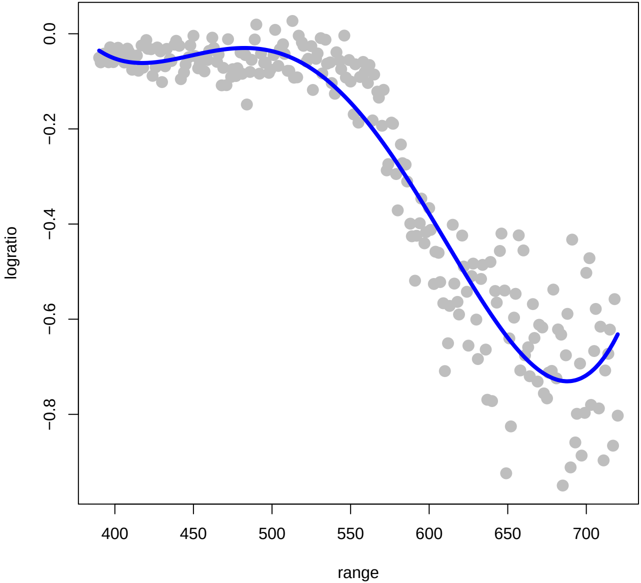
Non-linear regression

- Hence, we can try

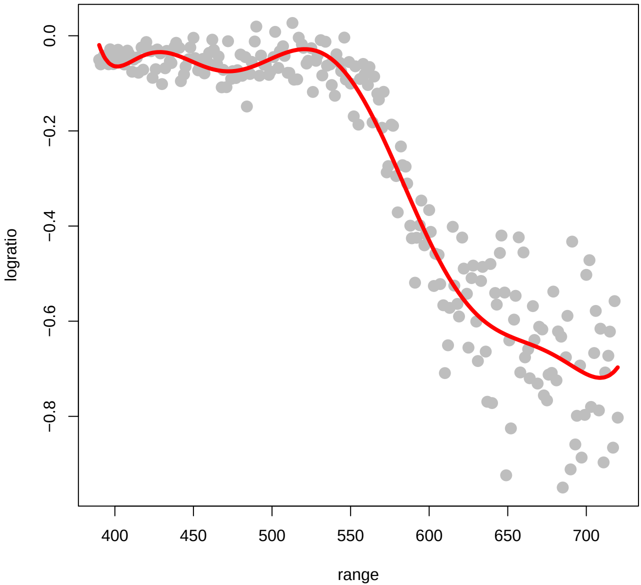
$$E[Y|X] = \beta_0 + \beta_1 X + \beta_2 X^2 + \ldots + \beta_k X^k$$

- This is a linear model! (**WHY?**)

LIDAR - 4th deg. polynomial



LIDAR - 10th deg. polynomial



More flexible bases

- Consider the (family) of function(s)

$$f_j(x) = \left(x - \kappa_j\right)_+ = \begin{cases} x - \kappa_j & \text{if } x - \kappa_j > 0 \\ 0 & \text{otherwise} \end{cases}$$

  where κ_j are *knots*

- Model

$$E\left[Y|\,X\right] = \beta_0 + \beta_1 X + \sum_{j=1}^{K} \beta_{j+1} f_j(X)$$

- This is a linear model

More flexible bases

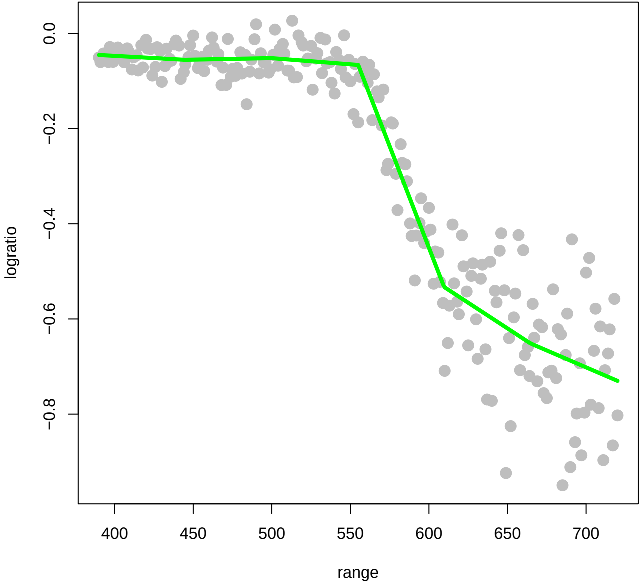
- The knots can be chosen arbitrarily
- It is customary to select them based on the sample

$$\kappa_j = \frac{j}{K+1} \, 100\% \text{ quantile of } x$$

- For example, with $K = 4$:

$$\kappa_1 = 20\% \,, \qquad \kappa_2 = 40\% \,, \qquad \text{etc.}$$

Regression splines, 5 knots



More flexible bases

- Consider a smoother basis

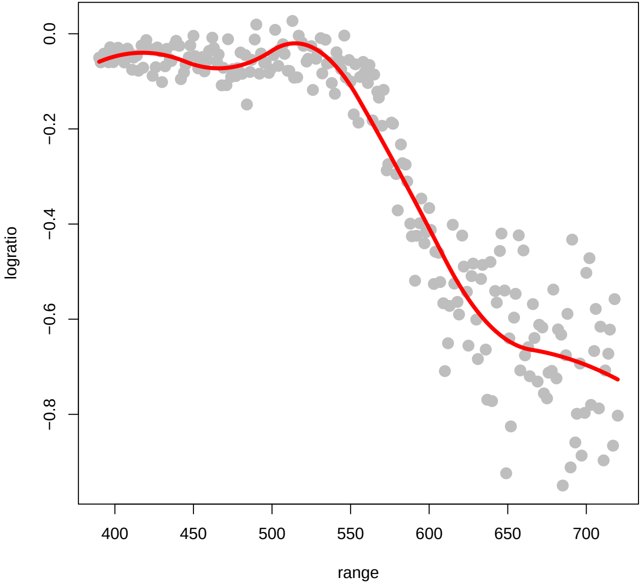
$$f_j(x) = \left(x - \kappa_j\right)_+^2 = \begin{cases} \left(x - \kappa_j\right)^2 & \text{if } x - \kappa_j > 0 \\ 0 & \text{otherwise} \end{cases}$$

  where κ_j, $1 \leq j \leq K$ are *knots*

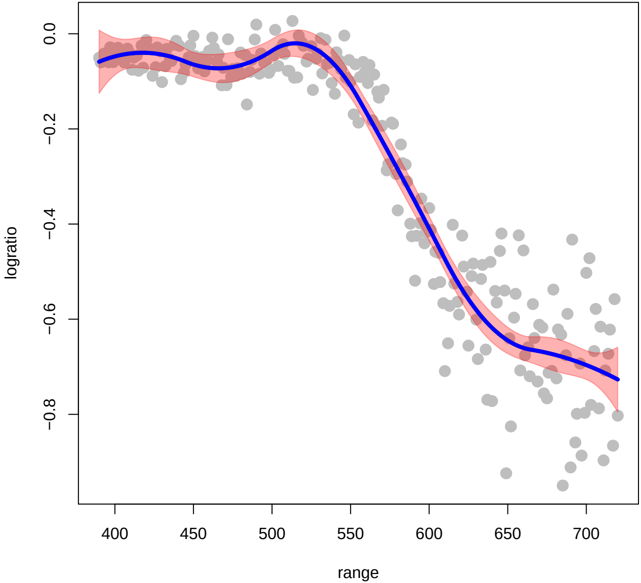
- Model

$$E\left[Y \mid X\right] = \beta_0 + \beta_1 X + \beta_2 X^2 + \sum_{j=1}^{K} \beta_{j+2} f_j(X)$$

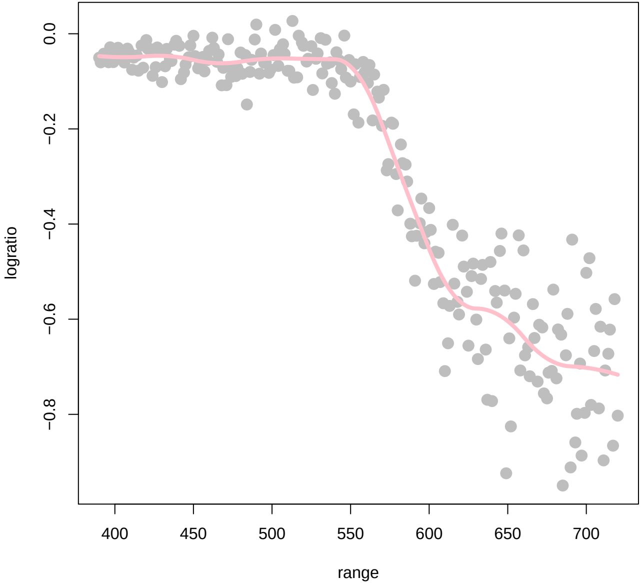
Quadratic splines, 5 knots



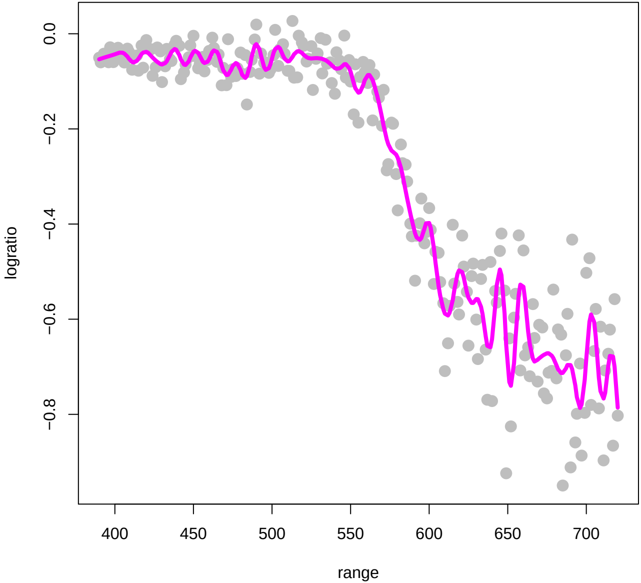
Quadratic splines, 5 knots + SEs



Quadratic splines, 10 knots



Quadratic splines, 50 knots



More flexible bases

- Cubic splines will be useful

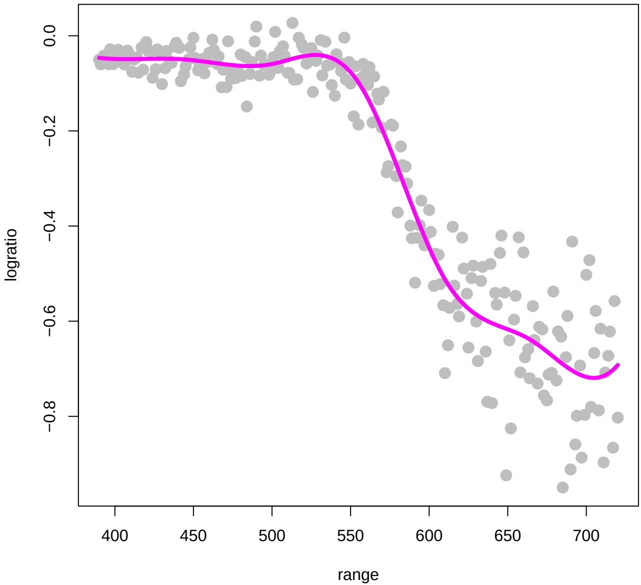
$$f_j(x) = \left(x - \kappa_j\right)_+^3 = \begin{cases} \left(x - \kappa_j\right)^3 & \text{if } x - \kappa_j > 0 \\ 0 & \text{otherwise} \end{cases}$$

where κ_j, $1 \le j \le K$ are *knots*

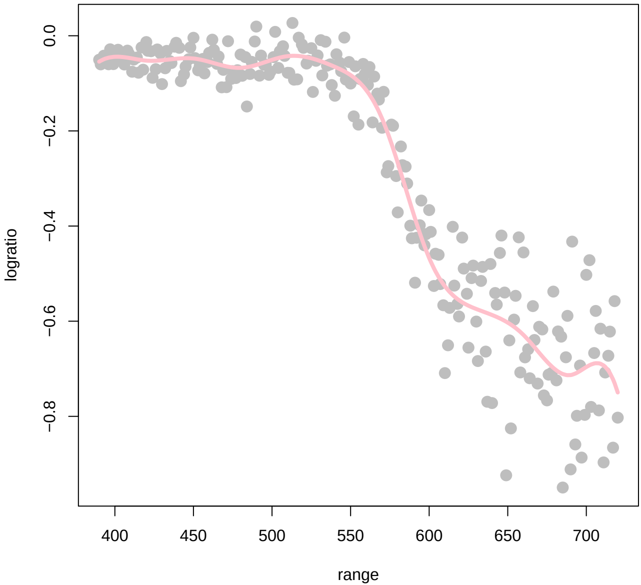
- Model

$$E\left[Y | X\right] = \beta_0 + \beta_1 X + \beta_2 X^2 + \beta_3 X^3 + \sum_{j=1}^{K} \beta_{j+3} f_j(X)$$

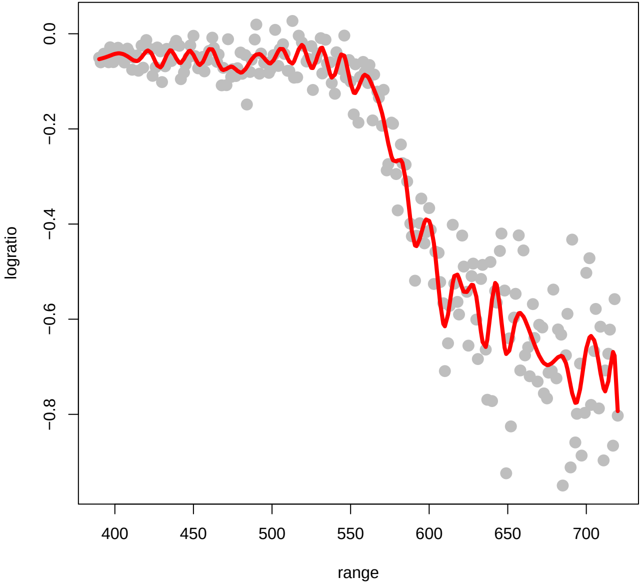
Cubic splines, 5 knots



Cubic splines, 10 knots



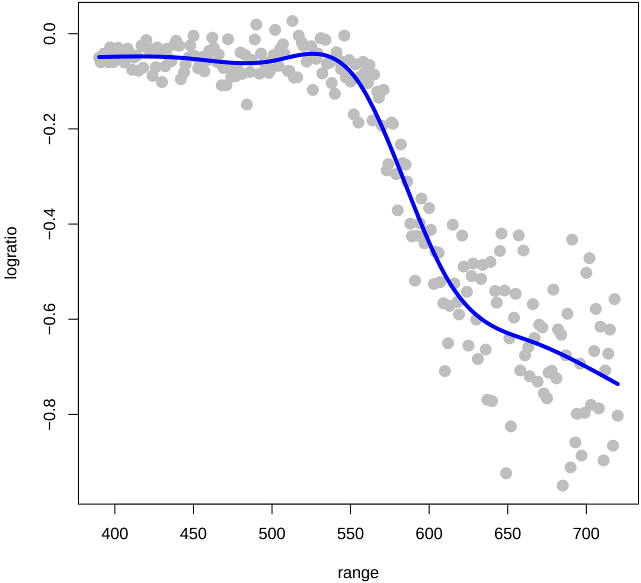
Cubic splines, 50 knots



More flexible bases

- Need to choose number and location of knots
- Need to make them less wiggly at the ends (Natural cubic splines)

Natural cubic spline, 5 knots



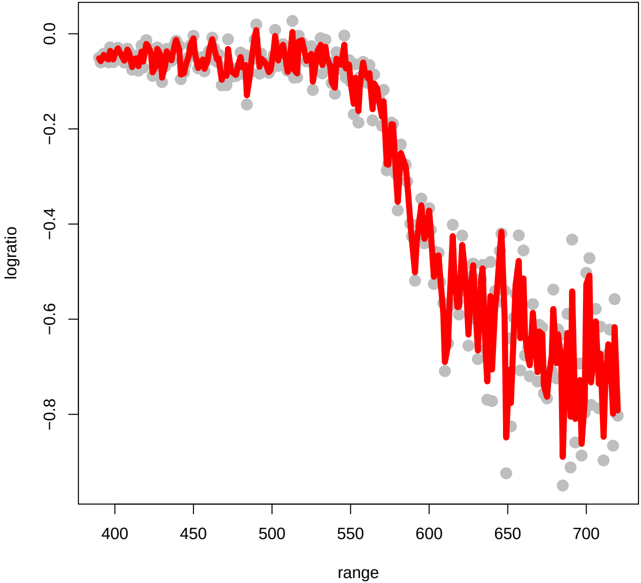
Smoothing splines

- Consider the following problem

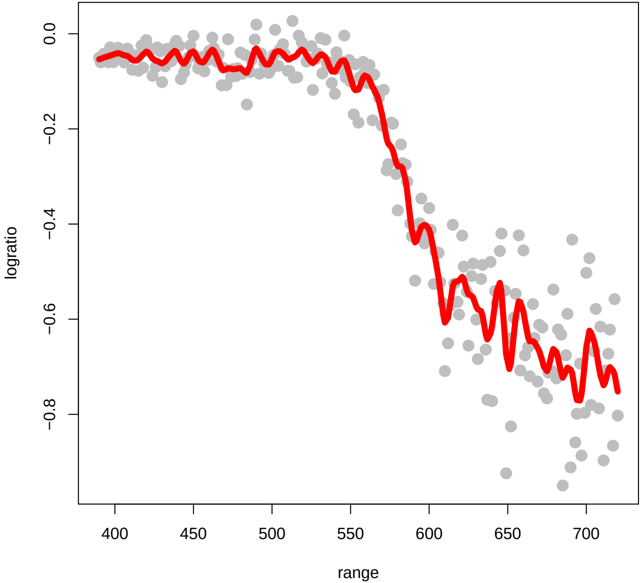
$$\min_{f} \sum_{i=1}^{n} (Y_i - f(X_i))^2 + \lambda \int \left(f^{(2)}(t) \right)^2 dt$$

- The solution is a *natural* cubic spline with n knots at $X_1, X_2, \ldots, X_n$.
- *Natural* cubic splines are cubic splines with the restriction that they are linear beyond the boundary knots.

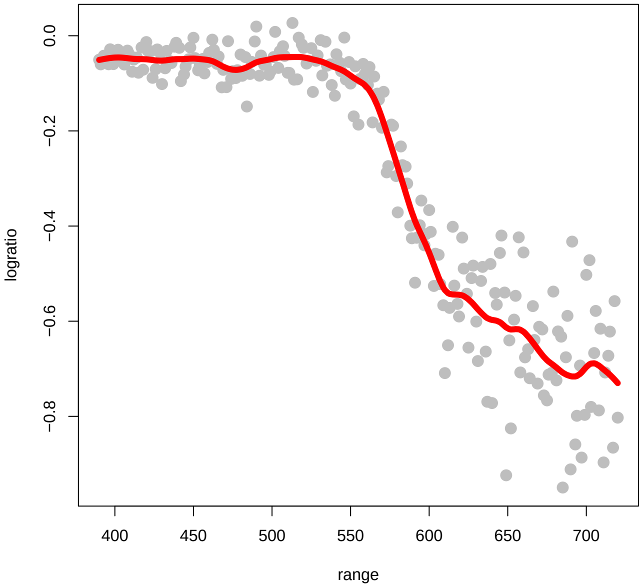
Smoothing spline, $\lambda = 0.20$



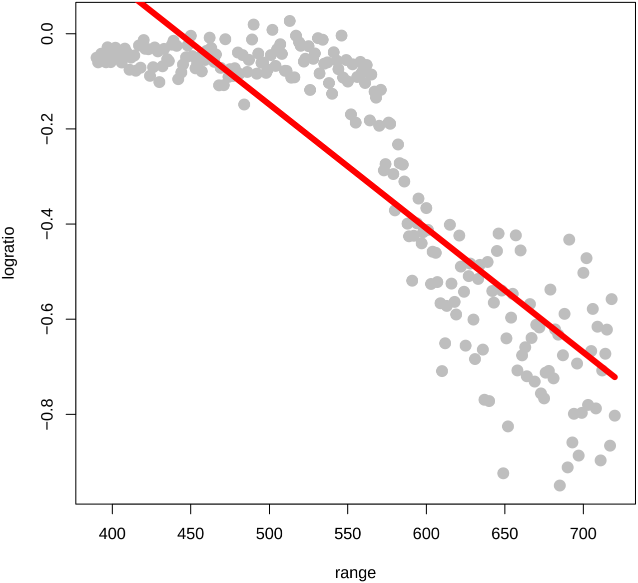
Smoothing spline, $\lambda = 0.50$



Smoothing spline, $\lambda = 0.75$



Smoothing spline, $\lambda = 2.00$



Selecting the penalty parameter

- How do we select λ?
- Minimizing

$$RSS(\lambda) = \sum_{i=1}^{n} (Y_i - \mathbf{X}_i' \beta_\lambda)^2$$

is not a good idea...

Selecting the penalty parameter

- Cross-validation: consider

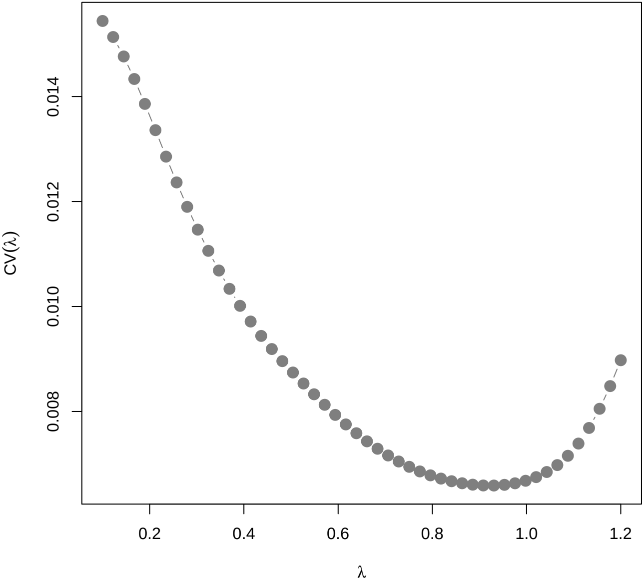
$$CV(\lambda) = \sum_{i=1}^{n} \left(Y_i - \mathbf{X}_i' \beta_\lambda^{(-i)} \right)^2$$

where $\beta_\lambda^{(-i)}$ is the fit without using the point (Y_i, X_i)

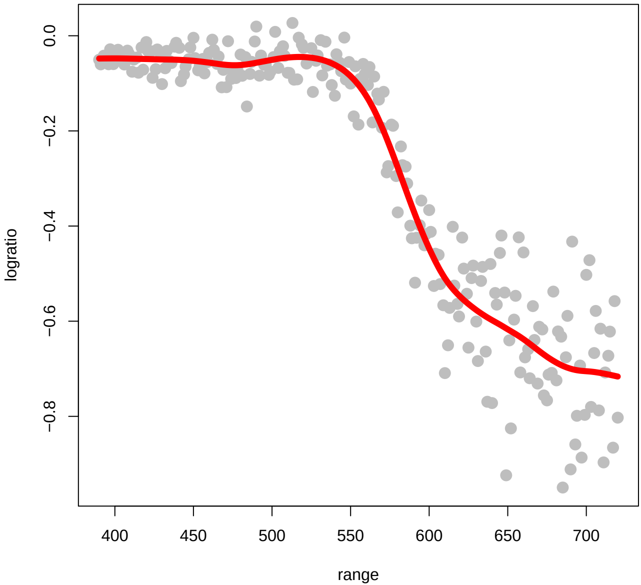
and choose a value λ_0 such that

$$CV(\lambda_0) \le CV(\lambda) \quad \forall \, \lambda \ge 0$$

5-fold CV, smoothing spline



Optimal fit via 5-fold CV



Selecting the penalty parameter

- Computing leave-one-out CV

$$CV(\lambda) = \sum_{i=1}^{n} \left(Y_i - \mathbf{X}_i' \beta_\lambda^{(-i)} \right)^2$$

We might need to re-fit the model n times

Selecting the penalty parameter

- For some smoothers and models this is not necessary. For many linear smoothers $\hat{\mathbf{Y}} = \mathbf{S}_\lambda \mathbf{Y}$ we have

$$\hat{\mathbf{Y}}_r = \sum_{i=1}^{n} \mathbf{S}_{\lambda,r,i} Y_i \qquad r = 1, \ldots, n$$

and then

$$\hat{\mathbf{Y}}_r^{(-r)} = \frac{\sum_{i \neq r} \mathbf{S}_{\lambda,r,i} Y_i}{\sum_{i \neq r} \mathbf{S}_{\lambda,r,i}}$$

Selecting the penalty parameter

- Furthermore

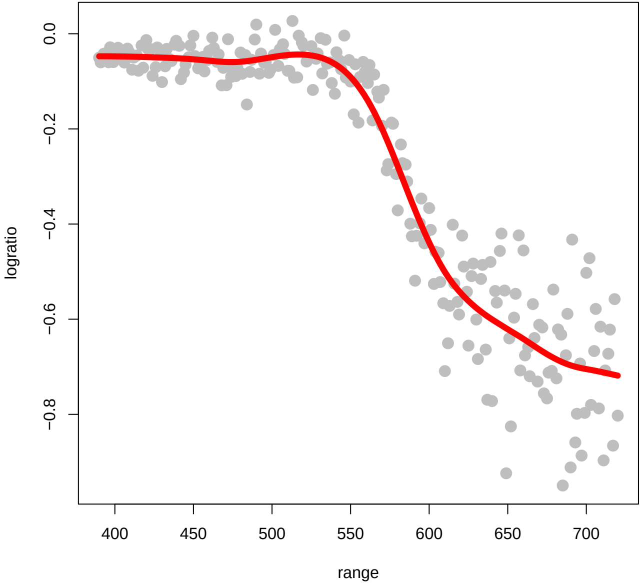
$$\mathbf{S}_\lambda \, \mathbf{1} = \mathbf{1}$$

thus

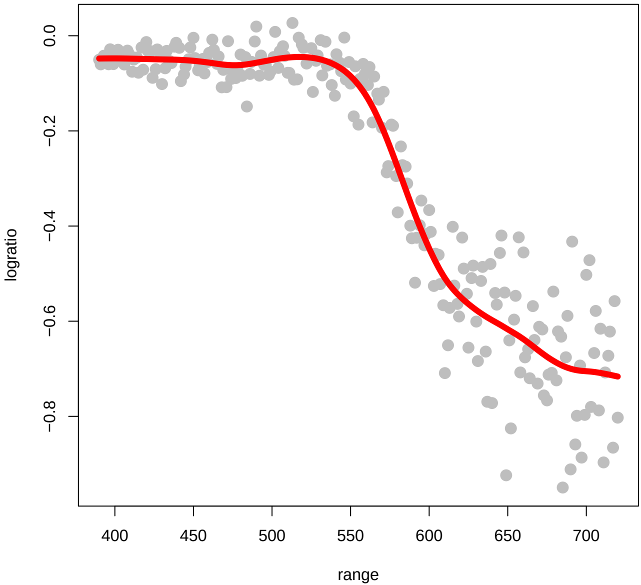
$$\hat{\mathbf{Y}}_r^{(-r)} = \frac{\sum_{i \neq r} \mathbf{S}_{\lambda,r,i} Y_i}{1 - \mathbf{S}_{\lambda,r,r}}$$

$$CV(\lambda) = \sum_{i=1}^{n} \left(\frac{Y_i - \hat{\mathbf{Y}}_i}{1 - \mathbf{S}_{\lambda,i,i}} \right)^2$$

Optimal fit via leave-1-out CV



Compare with 5-fold CV optimal



Selecting the penalty parameter

- Computing $\mathbf{S}_{\lambda,i,i}$, $i = 1, \ldots, n$ can be demanding

$$GCV(\lambda) = \sum_{i=1}^{n} \left(\frac{Y_i - \hat{\mathbf{Y}}_i}{1 - \mathrm{tr}(\mathbf{S}_\lambda)/n} \right)^2 =$$

$$= \frac{\sum_{i=1}^{n} \left(Y_i - \hat{\mathbf{Y}}_i \right)^2}{\left(1 - \mathrm{tr}(\mathbf{S}_\lambda)/n\right)^2}$$