

# Monotone Splines for Regression

## 1 The Regression Problem

Given some statistical data  $\{(x_i, y_i)\}_{i=1}^n$  where  $x_i, y_i \in \mathbb{R}$ , the regression problem is the problem of estimating the function  $f(x) = E(y|x)$  where  $f: \mathbb{R} \rightarrow \mathbb{R}$ . The primary difficulty here is to avoid overfitting, that is, to construct an estimate  $\hat{f}$  for the unknown function  $f$  that is close in some sense, not merely one that is close for the observed data points. This is the generalization problem. A good estimate  $\hat{f}$  is close to  $f$  even for non-observed values of  $x$ . To find such an estimate, we have make some prior assumptions about  $\hat{f}$ . These are typically enforced by either restricting the function class  $V$  from which we choose  $\hat{f}$  or by penalizing certain functions. Linear regression is an example of an extremely strong limitation on the class of functions used, viz.  $V = \{f: f(x) = ax + b\}$ . Here we use monotone splines (M-splines), integrated splines (I-splines), and convex splines (C-splines) as ways of restricting the class of functions to avoid overfitting.

## 2 Monotone Splines

We first a degree  $k$  for the spline function  $\hat{f}$  and a closed interval  $[a, b]$  for the domain of  $\hat{f}$ . This can be done, for instance, by using the minimum and maximum value of the set  $\{x_i\}$ . We then choose  $m$  interior break points  $t_{k+1}, \dots, t_{k+m} \in (a, b)$ . Lastly, define  $k$  additional break points at each end point  $t_1 = \dots = t_k = a$  and  $t_{m+k+1} = \dots = t_{m+2k} = b$  for notational simplicity.

The monotone splines or M-splines of order  $k$  are given by the recursive formula

$$\begin{aligned} M_i^{(1)}(x) &= \frac{\mathbb{1}_{[t_i, t_{i+1}]} }{t_{i+1} - t_i} \text{ if } t_{i+1} \neq t_i \\ M_i^{(1)}(x) &= 0 \text{ if } t_{i+1} = t_i \\ M_i^{(k)}(x) &= \frac{k[(x - t_i)M_i^{(k-1)}(x) + (t_{i+k} - x)M_{i+1}^{(k-1)}(x)]}{(k-1)} \end{aligned}$$

and then integrated and convex splines are defined by

$$\begin{aligned} I_i^{(k)}(x) &= \int_a^x M_i^{(k)}(t) dt \\ C_i^{(k)}(x) &= \int_a^x I_i^{(k)}(t) dt \end{aligned}$$

## 3 Degree $k = 1$

$t$

## 4 Degree $k = 2$

For  $i = 1$ :

$$M_1^{(2)}(x) = \begin{cases} 0, & x \notin [t_i, t_{i+2}] \\ \frac{2(x-t_i)}{(t_{i+2}-t_i)(t_{i+1}-t_i)}, & x \in [t_i, t_{i+1}] \\ \frac{-2(x-t_{i+2})}{(t_{i+2}-t_i)(t_{i+2}-t_{i+1})}, & x \in [t_{i+1}, t_{i+2}] \end{cases}$$

For  $i = 2, \dots, k + m - 1$ :

$$M_i^{(2)}(x) = \begin{cases} 0, & x \notin [t_i, t_{i+2}] \\ \frac{2(x-t_i)}{(t_{i+2}-t_i)(t_{i+1}-t_i)}, & x \in [t_i, t_{i+1}] \\ \frac{-2(x-t_{i+2})}{(t_{i+2}-t_i)(t_{i+2}-t_{i+1})}, & x \in [t_{i+1}, t_{i+2}] \end{cases}$$

## 5 Degree $k = 3$

## 6 Cubic Smoothing Splines

Given a set of points  $\{(x_i, y_i)\}_{i=1}^n$  and the spline order  $k = 4$ , we let the interior knots be given by  $(x_1, x_2, \dots, x_n)$ , add two boundary knots  $\xi_0$  and  $\xi_{n+1}$  for the end points of the domain, and then augment the knot sequence with  $k = 4$  redundant boundary knots on both sides of the interval, giving the final knot sequence as

$$(\xi_0, \xi_0, \xi_0, \xi_0, x_1, \dots, x_n, \xi_{n+1}, \xi_{n+1}, \xi_{n+1}, \xi_{n+1})$$