

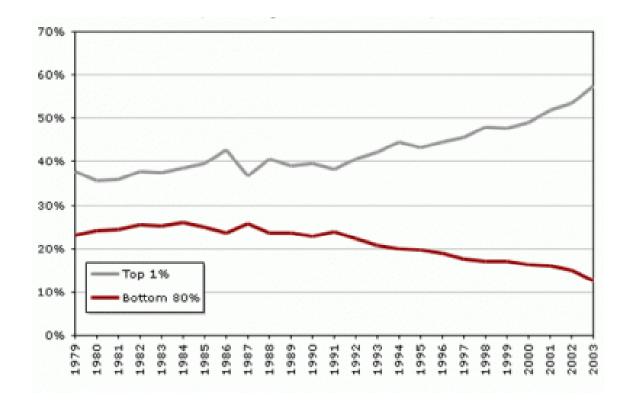
#### Average derivative estimation (1)

 In mean regression, we focus on estimating the conditional mean

 $\mu(\mathbf{x}) = E(Y|\mathbf{x})$ 

- In linear regression, the partial derivatives  $\partial \mu(\dot{\mathbf{x}})/\partial x_i$  are assumed to be constant.
- They are of primary interest because they measure how much the mean response change as the *i*th covariate perturb one unit.

### Average derivative estimation (2) Rich got richer, poor got poorer?



Share of capital income earned by top 1% and bottom 80%, 1979-2003 (Shapiro and Friedman 2006)

#### Average derivative estimation (3)

 For quantile regression, we may consider the average gradient

$$\beta_{\alpha} = (\beta_{\alpha 1}, \ldots, \beta_{\alpha d}) = E(\nabla \theta_{\alpha}(\mathbf{X}))$$

where  $\theta_{\alpha}(\mathbf{X})$  is the conditional  $\alpha$ th of Y given **X** 

#### Average derivative estimation (4)

Consider the model

 $Y = \mu(\mathbf{X}) + \tau [\mu(\mathbf{X})]^{\lambda} \varepsilon$ 

- ${m arepsilon}$  and  ${f X}$  are independent
- $\varepsilon$  has continuous distribution function  $F_{\varepsilon}$ the mean of  $\varepsilon$  is zero
- $\tau$  and  $\lambda$  are real parameters

#### Average derivative estimation (5)

• Let  $e_{\alpha}$  be the  $\alpha$ th quantile of  $F_{\varepsilon}$ 

$$\theta_{\alpha}(\mathbf{x}) = \mu(\mathbf{x}) + \tau [\mu(\mathbf{x})]^{\lambda} e_{\alpha}$$
  

$$\nabla \theta_{\alpha}(\mathbf{x}) = \nabla \mu(\mathbf{x}) + \tau \lambda [\mu(\mathbf{x})]^{\lambda - 1} \nabla_{\mu}(\mathbf{x}) e_{\alpha}$$
  

$$\beta_{\alpha} = E(\nabla \mu(\mathbf{X})) + \tau \lambda E \{ [\mu(\mathbf{X})]^{\lambda - 1} \nabla \mu(\mathbf{X}) \} e_{\alpha}$$

• If assuming 
$$F_{\varepsilon} = \Phi$$
  
 $d = \tau = \lambda = 1$   
 $\mu(x) = \gamma_1 + \gamma_2 x$   
then  
 $\beta_{\alpha} = [1 + \Phi^{-1}(\alpha)]\gamma_2$ 

 $\beta_{0.1} = -0.282\gamma_2, \qquad \beta_{0.5} = \gamma_2, \qquad \beta_{0.9} = 2.282\gamma_2$ 

# Average derivative estimation (6)

• Taking derivative on both side of the above equation and taking expectation, we get

$$E(\omega(\boldsymbol{X})\nabla\theta_{\alpha}(\boldsymbol{X})) = \left[\int g'(\gamma^{t}\boldsymbol{x})\omega(\boldsymbol{x})f(\boldsymbol{x})d\boldsymbol{x}\right]\gamma$$
$$= \beta\gamma$$

# Average derivative estimation (7)

• We may estimate

$$E(\omega(\boldsymbol{X})\nabla\theta_{\alpha}(\boldsymbol{X})) = \int \nabla\theta_{\alpha}(\boldsymbol{X})\omega(\boldsymbol{x})f(\boldsymbol{x})d\boldsymbol{x}$$

by  $\hat{\beta}_1 = n^{-1} \sum \{ \nabla \hat{\theta}(\mathbf{X}_i) \} w(\mathbf{X}_i)$ ,

where  $\nabla \hat{\theta}(\mathbf{X}_i)$  is a nonparametric estimator of the gradient of the conditional quantile  $\theta(\mathbf{x})$ 

# Average derivative estimation (8)

• By integration by parts,

$$\begin{split} E(\omega(\boldsymbol{X})\nabla\theta_{\alpha}(\boldsymbol{X})) &= \int \nabla\theta_{\alpha}(\boldsymbol{X})\omega(\boldsymbol{x})f(\boldsymbol{x})d\boldsymbol{x} \\ &= -\int \theta_{\alpha}(\boldsymbol{X})\nabla\{\omega(\boldsymbol{x})f(\boldsymbol{x})\}d\boldsymbol{x} \end{split}$$

• An alternative estimator is

$$\hat{\beta}_{2} = -\frac{1}{n} \sum_{i=1}^{n} \hat{\theta}(\mathbf{X}_{i}) \frac{\nabla w(\mathbf{X}_{i}) \hat{f}(\mathbf{X}_{i}) + w(\mathbf{X}_{i}) \nabla \hat{f}(\mathbf{X}_{i})}{\hat{f}(\mathbf{X}_{i})}$$
$$= -\frac{1}{n} \sum_{i=1}^{n} \hat{\theta}(\mathbf{X}_{i}) \Big\{ \nabla w(\mathbf{X}_{i}) + w(\mathbf{X}_{i}) \hat{\ell}(\mathbf{X}_{i}) \Big\},$$

where  $\hat{\ell}(\mathbf{X}_i) = \nabla \hat{f}(\mathbf{X}_i) / \hat{f}(\mathbf{X}_i)$ ,  $\hat{f}$  and  $\nabla \hat{f}$  are nonparametric estimator of the density and its derivative

# Average derivative estimation (9)

Leave one out estimator

$$\hat{f}(\mathbf{X}_i) = \frac{1}{(n-1)h_n^d} \sum_{j \neq i} W\left(\frac{\mathbf{X}_j - \mathbf{X}_i}{h_n}\right),$$

$$\nabla \hat{f}(\mathbf{X}_i) = \frac{1}{(n-1)h_n^{d+1}} \sum_{j \neq i} W^{(1)} \left( \frac{\mathbf{X}_j - \mathbf{X}_i}{h_n} \right),$$

#### Penalized univariate smoothing method (1)

Assume that

$$y = f(x) + \epsilon$$

• In case of the mean regression, we may consider estimate the function f by minimizing

$$RSS(f,\lambda) = \sum_{i=1}^{N} \{y_i - f(x_i)\}^2 + \lambda \int \{f''(t)\}^2 dt,$$

 $\lambda=0:\ f$  can be any function that interpolates the data.

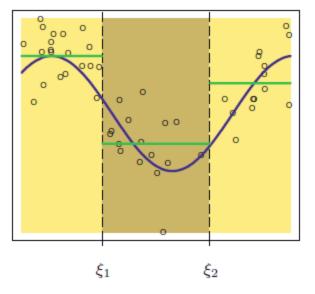
 $\lambda = \infty$  : the simple least squares line fit, since no second derivative can be tolerated.

• It can be shown that for  $\lambda \in (0,\infty)$ , there is a unique minimizer, which is a natural cubic spline with knots at  $x_i$ 

### Splines (1)

- Suppose that we can to estimate a function f(.) with a piecewise polynomial function
- In the simplest case, we can just estimate f by a piecewise constant function
- We may write

$$f(X) = \sum_{m=1}^{3} \beta_m h_m(X)$$
$$h_1(X) = I(X < \xi_1),$$
$$h_2(X) = I(\xi_1 \le X < \xi_2),$$
$$h_3(X) = I(\xi_2 \le X).$$



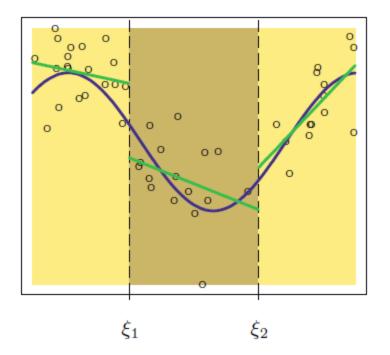
Piecewise Constant

### Splines (2)

• We may also fit f by a piecewise linear function, which requires 3 additional base function

$$h_{m+3} = h_m(X)X, \ m = 1, \dots, 3$$

Piecewise Linear

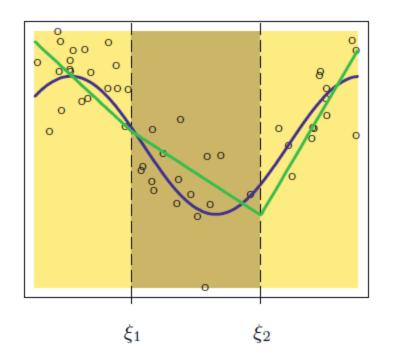


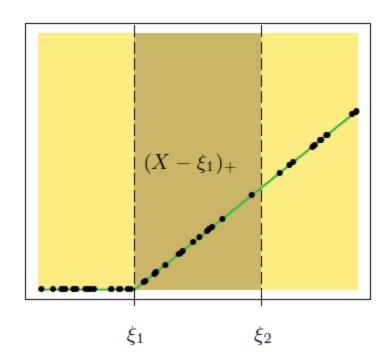
# Splines (3)

 If we require continuity on the knots, we put some constraints (2 constraints in the above exmple) on the coefficient of

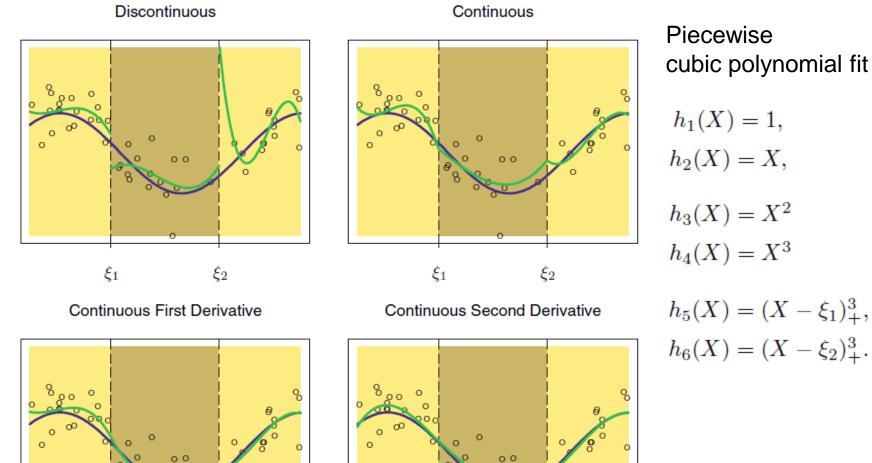
$$f(X) = \sum_{m=1}^{M} \beta_m h_m(X),$$

• More conveniently, we may write the base functions





# Splines (4)



ξ1

 $\xi_2$ 

ξı

 $\xi_2$ 

cubic polynomial fit

### Splines (5)

- An order-M spline with knots ξ<sub>j</sub>, j = 1,...,K is a piecewise-polynomial of order M (degree M-1), has continuous derivative up to order M-2
- A cubic spline has order M=4
- The bases are

$$h_j(X) = X^{j-1}, \ j = 1, \dots, M,$$
  
$$h_{M+\ell}(X) = (X - \xi_\ell)_+^{M-1}, \ \ell = 1, \dots, K.$$

#### Natural cubic splines

- In addition to requiring the function to have continuous derivatives on the knots, we require the function is linear beyond the boundary points
- If the function is represented as

$$f(X) = \sum_{j=0}^{3} \beta_j X^j + \sum_{k=1}^{K} \theta_k (X - \xi_k)_+^3.$$

it can be shown that

$$\beta_2 = 0, \qquad \sum_{k=1}^{K} \theta_k = 0, \\ \beta_3 = 0, \qquad \sum_{k=1}^{K} \xi_k \theta_k = 0.$$

#### B-splines (1)

Let 
$$\xi_0 < \xi_1$$
 and  $\xi_K < \xi_{K+1}$  be two boundary knots,  
 $\tau_1 \le \tau_2 \le \cdots \le \tau_M \le \xi_0;$   
 $\tau_{j+M} = \xi_j, \ j = 1, \cdots, K;$   
 $\xi_{K+1} \le \tau_{K+M+1} \le \tau_{K+M+2} \le \cdots \le \tau_{K+2M}.$ 

$$B_{i,1}(x) = \begin{cases} 1 & \text{if } \tau_i \le x < \tau_{i+1} \\ 0 & \text{otherwise} \end{cases}$$

for  $i = 1, \dots, K + 2M - 1$ .

$$B_{i,m}(x) = \frac{x - \tau_i}{\tau_{i+m-1} - \tau_i} B_{i,m-1}(x) + \frac{\tau_{i+m} - x}{\tau_{i+m} - \tau_{i+1}} B_{i+1,m-1}(x)$$
  
for  $i = 1, \dots, K + 2M - m$ .

#### B-splines (2)

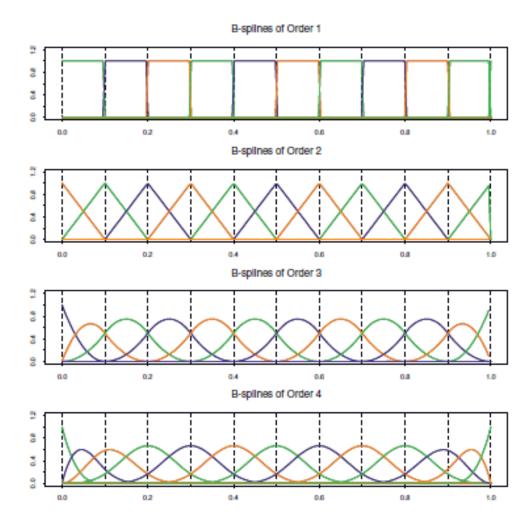


FIGURE 5.20. The sequence of B-splines up to order four with ten knots evenly spaced from 0 to 1. The B-splines have local support; they are nonzero on an interval spanned by M + 1 knots.

# Quantile regression-penalized method (1)

• For quantile regression, we may consider

$$\min_{g \in \mathcal{G}} \sum_{i=1}^n \rho_\tau(y_i - g(x_i)) + \lambda \int (g''(x))^2 dx.$$

• The solution is also a natural cubic spline

# Quantile regression-penalized method (2)

Koenker, Ng, and Portnoy (1994) consider other  $L_p$  penalties

$$J(g) = \|g''\|_p = (\int (g''(x))^p)^{1/p}.$$

For p = 1

$$\min\sum_{i=1}^n \rho_\tau(y_i - g(x_i)) + \lambda \int |g''(x)| dx$$

# Quantile regression-penalized method (3)

- Another way to penalize the objective function is P(g) = V(g')
- The total variation is defined as  $V(f) = \sup \sum_{i=1}^{n} |f(x_{i+1}) - f(x_i)|,$

where the sup is taken over all partitions  $a \le x_1 < \cdots < x_n < b$ 

• For absolute continuous function

$$V(f) = \int_{a}^{b} |f'(x)| dx$$

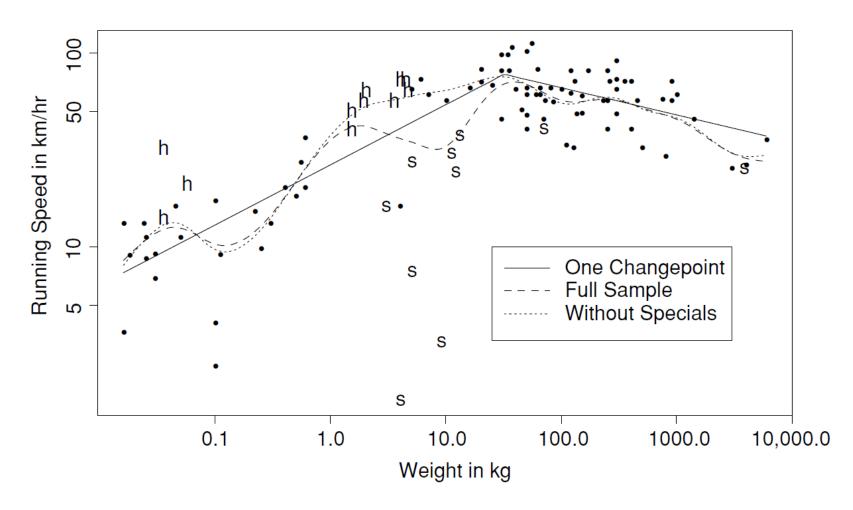
# Quantile regression-penalized method (4)

• The new penalized objective function is

$$\min_{g \in \mathcal{G}} \sum_{i=1}^{n} \rho_{\tau}(y_i - g(x_i)) + \lambda V(g')$$

• The solution is a piecewise linear function

# Animal weight VS running speed



#### h: hoppers

s: specials including sloth, porcupine, hippopotamus