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Quantile smoothing splines

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Summary

Although nonparametric regression has traditionally focused on the estimation of conditional mean functions, nonparametric estimation of conditional quantile functions is often of substantial practical interest. We explore a class of quantile smoothing splines, defined as solutions to

$$\min_{g \in \mathscr{G}} \sum \rho_\tau\{y_i - g(x_i)\} + \lambda \left(\int_0^1 |g''(x)|^p \, dx \right)^{1/p},$$

with $\rho_\tau(u) = u\{\tau - I(u < 0)\}$, $p \geqslant 1$, and appropriately chosen $\mathscr{G}$. For the particular choices $p = 1$ and $p = \infty$ we characterise solutions $\hat{g}$ as splines, and discuss computation by standard l_1-type linear programming techniques. At $\lambda = 0$, $\hat{g}$ interpolates the τth quantiles at the distinct design points, and for λ sufficiently large $\hat{g}$ is the linear regression quantile fit (Koenker & Bassett, 1978) to the observations. Because the methods estimate conditional quantile functions they possess an inherent robustness to extreme observations in the y_i's. The entire path of solutions, in the quantile parameter τ, or the penalty parameter λ, may be efficiently computed by parametric linear programming methods. We note that the approach may be easily adapted to impose monotonicity and/or convexity constraints on the fitted function. An example is provided to illustrate the use of the proposed methods.

Some key words: Bandwidth selection; Nonparametric regression; Quantile; Smoothing; Spline.

1. Introduction

Several authors have recently proposed methods for nonparametric estimation of conditional quantile functions: Truong (1989) following the pioneering work of Stone (1977) on nearest neighbour methods; Antoch & Janssen (1989), Samanta (1989), Bhattacharya & Gangopadhyay (1990) and Chaudhuri (1991), using kernel methods; Cole & Green (1992) applying a penalised likelihood approach; and White (1990) employing neural networks. Hendricks & Koenker (1992) discuss regression spline models and apply them to electricity demand data. Cox & Jones in the discussion of Cole (1988), reviving a suggestion of Bloomfield & Steiger (1983), have recently proposed estimating quantile smoothing splines which minimise

$$\sum_{i=1}^{n} \rho_\tau\{y_i - g(x_i)\} + \lambda \int \{g''(x)\}^2\, dx, \qquad (1\cdot 1)$$

where $\rho_\tau(u) = u\{\tau - I(u<0)\}$ is the check function of Koenker & Bassett (1978). Here the parameter $\tau \in [0, 1]$ controls the quantile of interest, while $\lambda \in \mathbb{R}_+$ controls the smoothness of the resulting cubic spline, thus generalising the extensive literature on classical least squares smoothing splines pioneered by Wahba (1990). This is an intriguing idea, and has also been mentioned, for example, by Cox (1983), Eubank (1988, p. 294) and Utreras (1981) in the median $\rho_{\frac{1}{2}}(u) = \frac{1}{2}|u|$ case. However, the resulting quadratic program poses some serious computational obstacles. A recent paper by Bosch, Ye & Woodworth (1994) discusses an interior point algorithm for this problem. Obviously the computational virtues of the piecewise linear form of the first term of the objective function are sacrificed by the quadratic form of the smoothness penalty.

One is thus led to consider replacing $\{g''(x)\}^2$ in the penalty by $|g''(x)|$. The median special case of this problem has been studied by Schuette (1978). We will show, expanding on Schuette's discrete version of the problem using finite differences, that minimising (2·1) below retains the linear programming form of the parametric version of the quantile regression problem and yields solutions which are easy to compute. Solutions with this L_1 form of the roughness penalty are linear splines and therefore provide a natural, automatic approach to estimating certain piecewise linear change-point models. An application to the relationship between maximal running speed and body mass of terrestrial mammals is provided in § 3. It should be noted that these quantile smoothing splines achieve the usual $n^{-2/5}$ rate of convergence when the true regression quantile function is twice continuously differentiable. A formal statement of this convergence in the L_2 norm is given in recent work by Xiaotong Shen.

2. Quantile smoothing splines

2·1. *The L_1 roughness penalty*

In prior work (Koenker, Ng & Portnoy, 1992), we have considered the problem of minimising

$$R_{\tau,\lambda}(g) = \sum_{i=1}^{n} \rho_\tau\{y_i - g(x_i)\} + \lambda \int_0^1 |g''(x)|\, dx, \qquad (2\cdot 1)$$

with $0 = x_0 < x_1 < \ldots x_n < x_{n+1} = 1$, over the Sobolev space W_1^2 of continuous functions on $[0, 1]$ with absolutely continuous first derivative and absolutely integrable second derivative. However, the argument given there that the solution to (2·1) is a parabolic spline, i.e. piecewise quadratic, is incorrect. Indeed the problem expressed in (2·1) is ill posed since the infimum of $R_{\tau,\lambda}$ is not attained by an element of W_1^2. The situation can be rectified by reformulating the problem somewhat, adopting the approach of Fisher & Jerome (1975) and Pinkus (1988) who consider closely related problems of optimal interpolation.

We begin by briefly reviewing some results on optimal interpolation. For an integer $k \geqslant 2$ and $p \in [1, \infty)$, let $\|f\|_p = (|f(x)|^p)^{1/p}$ and let W_p^k denote the Sobolev space of real functions on $[0, 1]$ with $k-1$ absolutely continuous derivatives and kth derivative existing almost everywhere as a function in $L_p[0, 1]$. We wish to find the smoothest interpolant of the points $\{(x_i, y_i), i = 1, \ldots, n\}$ in the sense of solving

$$\inf\{\|g^{(k)}\|_p : g \in W_p^k, g(x_i) = y_i, i = 1, \ldots, n\}. \tag{2·2}$$

The case $p = 2$ is best known, yielding splines of degree $2k - 1$ with knots at the points $\{x_i, i = 1, \ldots, n\}$. We are primarily interested in the case of $p = 1$ which has been treated by Fisher & Jerome (1975) and Pinkus (1988).

For $p = 1$, apparently Fisher & Jerome (1975) were the first to observe that (2·2) has no solution for $g \in W_1^k$. They showed that, if W_1^k is expanded to include functions whose kth derivatives are measures, the expanded problem does have a solution s, as a spline of degree $k - 1$, that the total variation of its $(k-1)$th derivative, $V(s^{(k-1)})$, coincides with the extremal value of (2·2), and that the measure $s^{(k)}$ is concentrated on n or fewer points. Pinkus (1988) has refined this characterisation somewhat and has provided considerable further generalisation. To bridge the gap between the smoothing problem posed in (2·1) and the optimal interpolation problem (2·2), we observe that any solution, $\hat{g}$, must interpolate itself at the observed $\{x_i\}$ and therefore must minimise the roughness penalty, subject to a given fidelity constraint. Thus to determine the form of the solution to the smoothing problem it suffices to consider the interpolation problem.

It remains to consider the question of knot selection for the $p = 1$ case. Pinkus (1988), under somewhat restrictive conditions on the y_i's, notes that for $k = 2$, the case of primary interest here, the knots of the optimal spline coincide with the observed x_i. That this is true for any configuration of y_i's can be argued as follows. Let f by any interpolator of the points $\{(x_i, y_i): i = 1, \ldots, n\}$ with an absolutely continuous first derivative. Recall, e.g. Natanson (1974, p. 259), that the total variation of an absolutely continuous function is the integral of the absolute value of its derivative. Thus, by the mean value theorem, it is possible to choose $u_i \in (x_i, x_{i+1})$ such that

$$f'(u_i) = (y_{i+1} - y_i)/(x_{i+1} - x_i) \quad (i = 1, \ldots, n-1).$$

Then,

$$V(f') \geqslant \sum_{i=1}^{n-1} \left| \int_{u_i}^{u_i+1} f''(x)\, dx \right| \geqslant \sum_{i=1}^{n-1} |f'(u_{i+1}) - f'(u_i)| = V(\hat{f}'),$$

where $\hat{f}$ is the piecewise linear interpolator with knots at the x_i. Finally, note that for any continuous piecewise linear g there exists a sequence of functions $\{g_n\}$ with absolutely continuous first derivative such that $\lim V(g_n') = V(g')$, and thus by the foregoing argument $\hat{f}$ minimises $V(g)$ for all such g.

Thus, following Pinkus (1988) if we expand our original space slightly from the Sobolev space W_1^2 to

$$U^2 = \left\{ g : g(x) = a_0 + a_1 x + \int_0^1 (x - y)_+ \, d\mu(y),\ V(\mu) < \infty,\ a_i \in \mathbb{R},\ i = 0, 1 \right\}$$

and replace the L_1 penalty on g'' with a total variation penalty on g', we obtain the following.

THEOREM 1. *The function $g \in U^2$ minimising $\sum \rho_\tau\{y_i - g(x_i)\} + \lambda V(g')$ is a linear spline with knots at the points x_i $(i = 1, \ldots, n)$.*

Having established the form of the solution, it is straightforward to develop an algorithm to compute $\hat{g}$. We write $\hat{g}(x) = \alpha_i + \beta_i(x - x_i)$ for $x \in [x_i, x_{i+1})$ $(i = 0, \ldots, n)$. By the continuity of $\hat{g}$, $\beta_i = (\alpha_{i+1} - \alpha_i)/h_i$, where $h_i = x_{i+1} - x_i$. The penalty may thus be expressed as

$$V(\hat{g}') = \sum_{i=1}^{n-1} |\beta_{i+1} - \beta_i| = \sum_{i=1}^{n-1} |(\alpha_{i+2} - \alpha_{i+1})/h_{i+1} - (\alpha_{i+1} - \alpha_i)/h_i|.$$

Thus parameterising $\hat{g}$ by the n-vector $\alpha = (\hat{g}(x_i))$, we may write the original problem as a linear program:

$$\min_{\alpha \in \mathbb{R}^n} \sum_{i=1}^{n} \rho_\tau(y_i - \alpha_i) + \lambda \sum_{j=1}^{n-1} |d_j'\alpha|, \tag{2·3}$$

where

$$d_j' = (0, \ldots, 0, h_j^{-1}, -(h_{j+1}^{-1} + h_j^{-1}), h_{j+1}^{-1}, 0, \ldots, 0) \quad (j = 1, \ldots, n-1).$$

In the important special median case, $\tau = \frac{1}{2}$, we can view this as simple data augmentation and therefore as an ordinary least absolute deviation regression problem. For general τ, further modifications are conceptually straightforward. Details of an implementation in 'S' (Becker, Chambers & Wilks, 1988) are available from the authors on request. Since we have n free parameters α, and $2n-1$ pseudo-observations, solutions must have n zero pseudo-residuals by complementary slackness. And in our case these zeros correspond to either (i) exact interpolation of observations, so $\hat{\alpha}_i = y_i$, or (ii) linearity of $\hat{g}$ at an internal knot, that is $\beta_{i+1} = \beta_i$ for some index i. The parameter λ controls the comparative 'advantage' of these two alternative means of reducing the objective function. When λ is sufficiently large, all the $\hat{\beta}_i$ will be equal and the solution will be the bivariate linear quantile regression fit (Koenker & Bassett, 1978). When λ is sufficiently small, all n observations will be interpolated when the design points are unique, otherwise the τth quantiles at each distinct design point are interpolated.

2·2. *Bandwidth choice*

As in any smoothing problem, choice of 'bandwidth', here represented by the parameter λ, is critical. For quantile smoothing splines, the problem of computing a family of solutions for various λ is greatly eased by the fact that the problem is a parametric linear program in the parameter λ. This is an immediate consequence of the fact that the objective function is linear in λ. Geometrically, we may think of solving (2·3) as minimising a linear function in the α's, after the introduction of 'slack variables' to accommodate the piecewise linear form of the fidelity and penalty terms, subject to a polyhedral constraint set. As λ changes, the orientation of the linear function changes, and we move from one adjacent vertex of the constraint polytope to the next. Solutions $\hat{g}_{\tau,\lambda}(.)$ are thus piecewise constant in λ; that is there exists a mesh $0 = \lambda_0 < \lambda_1 < \ldots < \lambda_J$, such that $\hat{g}_{\tau,\lambda}$ solves (2·3) for all $\lambda \in [\lambda_{i-1}, \lambda_i]$. Based on our empirical experience, and the results of Portnoy (1991) for the closely related problem of the number of distinct solutions in τ to the linear quantile regression problem, the number of distinct solutions, J, in λ, could be conjectured to be $O_p(n \log n)$. An important consequence of this is that we may initially solve the much smaller linear quantile regression problem corresponding to $\lambda = \infty$ and gradually relax the roughness penalty with a sequence of simplex pivots, thus avoiding a direct solution of a potentially large problem.

Each transition to a new solution of the parametric linear program in λ involves a single simplex pivot of an extremely sparse tableau, and hence solving for a broad range of λ is quite efficient. The situation is analogous to the problem of solving for the entire family of quantile regression solutions in the parameter τ, described originally by Bassett & Koenker (1982), and in greater detail by Koenker & d'Orey (1987).

An interesting and important aspect of the way that solutions depend upon the penalty parameter λ involves the number of interpolated points. In the classical L_2 smoothing spline literature much has been made of the 'effective dimensionality' or 'degrees of freedom' of the estimated curves corresponding to various λ. Such measures are usually based on the trace of various quasi-projection matrices in the least squares theory; see, for example, Hastie & Tibshirani (1990, Ch. 3) for a cogent discussion. For the quantile smoothing spline the connection is more direct in the sense that there is an explicit trade-off between the number of interpolated points and the number of linear segments. If the design is in 'general position' so that no two observations share the same design point, the number p_λ of interpolated y_i's must be at least 2 and at most n. In effect, p_λ is the number of 'active' knots. Clearly, p_λ is a plausible measure of the effective dimension of the fitted model with penalty parameter λ, and $n-p_\lambda+1$, which corresponds to the number of linear segments in the fitted function, is a plausible measure of the degrees of freedom of the fit. Such decompositions may be used in conjunction with the function $R_{\tau,\lambda}(\hat{g})$ itself to implement data-driven bandwidth choice. The criterion

$$\mathrm{SIC}\,(p_\lambda)=\log\left[n^{-1}\sum_{i=1}^{n}\rho_\tau\{y_i-\hat{g}(x_i)\}\right]+\tfrac{1}{2}n^{-1}p_\lambda\log n, \qquad (2{\cdot}4)$$

which may be interpreted as the Schwarz (1978) criterion for the quantile smoothing spline problem, seems to perform well in some limited applications. Machado (1993) considers similar criteria for parametric quantile regression and more general M-estimators of regression.

2·3. *Extensions*

There is considerable scope for other forms of the roughness penalty. We have focused on the L_1 penalty on g'', but other L_p norms are possible as are other differential operators. From a computational point of view the L_∞ roughness penalty is also an attractive choice since it too yields a linear programming formulation. However, unlike the L_1 penalty, the L_∞ penalty produces a quadratic rather than a linear spline. The L_∞ penalty may be viewed as a uniform prior on g'', with each λ implying a corresponding upper bound on $\sup|g''(x)|$.

To extend these methods to multivariate settings the additive spline models of Hastie & Tibshirani (1990) and others suggest themselves. Some preliminary plots for bivariate x look quite promising. The nonlinear character of the present smoothers vitiate the attractive iterative 'backfitting' algorithms available in the L_2-case, but feasible estimators may still be possible using a limited number of simplex pivots from an initial linear-in-covariates quantile function estimate.

There are several intriguing extensions incorporating further constraints. Monotonicity and convexity of the fitted function $\hat{g}$ may be imposed via further linear inequality constraints on the parameters. While adding such inequality constraints to the corresponding L_2 problem results in a significant increase in complexity, adding linear inequality constraints to the quantile smoothing spline problems does not alter the fundamental nature of the optimisation problem to be solved.

3. An example

Our example, based on Chappell (1989), explores the relationship between maximal running speed and body mass of terrestrial mammals. The data, collected and described in detail by Garland (1983), are plotted in Fig. 1; 107 species are represented. Two groups are identified for special treatment by Chappell: 'hoppers' which, like the kangaroo, ambulate by hopping and are labelled by the plotting character h in the figure, and 'specialised', labelled s, which like the hippopotamus, the porcupine, and man 'were judged unsuitable for the inclusion in analyses on account of lifestyles in which speed does not figure as an important factor'. For reference we have included Chappell's single change-point log-linear model, estimated by least squares. It omits the s observations and fits an additive shift effect for the 'hoppers'. Superimposed in Fig. 1 we illustrate two cubic smoothing splines estimated by minimising the usual penalised least squares criterion. The dashed curve is the fit when the entire sample is included; the dotted curve excludes the special animals labelled s. In both cases λ is chosen by generalised crossvalidation as described, for example, by Craven & Wahba (1979). One can immediately see the lack of robustness of the least squares splines to the slower special animals.

Next we fit the entire family of median smoothing splines using the L_1 penalty. There are 182 distinct curves corresponding to λ's ranging from 0 to ∞. In Fig. 2 we plot 3 of these curves for $\lambda = \{1{\cdot}01, 12{\cdot}23, 41{\cdot}16\}$. The dimensions of the fitted functions represented by the number of interpolated points $\{10, 3, 2\}$ respectively are given in the legend. Like the least squares spline in Fig. 1, these estimates are based on all the observations. However, unlike the least squares splines which estimate the conditional mean function, these median splines have an inherent robustness to outliers in the vertical direction. As in parametric quantile regression, points may be moved up or down in the plot without affecting the fitted function so long as they do not cross it. This follows immediately from the fact that the subgradient of the objective function depends upon the y_i only through the signs of the residuals, not their magnitude. See Koenker & Bassett (1978, Theorem 3·5).

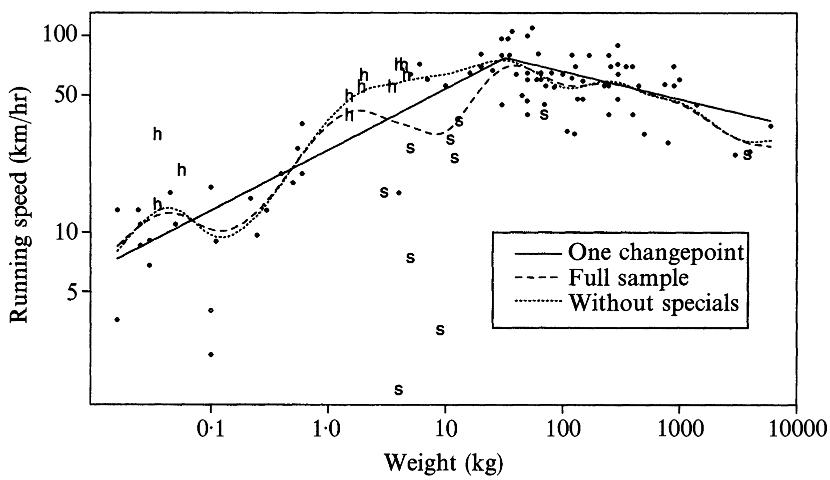

Fig. 1. Body mass versus maximal recorded running speed of 107 terrestrial mammals with estimated piecewise linear change-point model from Chappell (1989) and two least-squares smoothing splines.

Minimising SIC (p_λ) by (2·4) over λ selects the solid line with a single break. This fit is remarkably similar to Chappell's preferred single change-point model, especially consider-

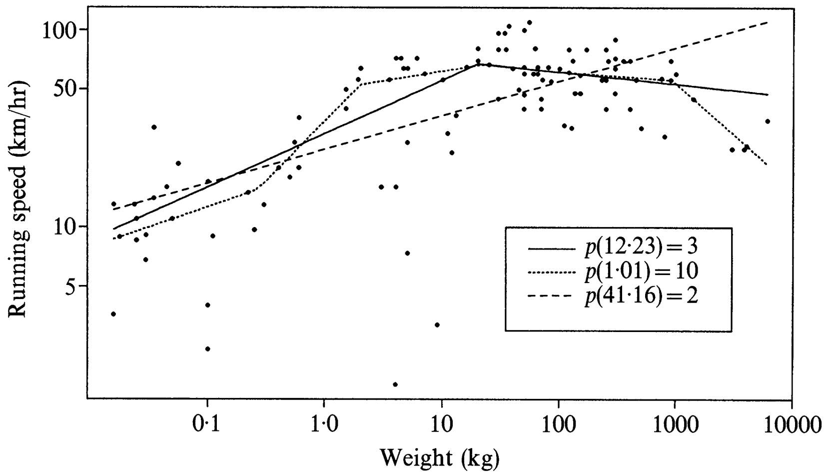

Fig. 2. Mammal data and three median L_1 smoothing splines: effective dimension of the splines is $p(\lambda)$ indicated by the legend.

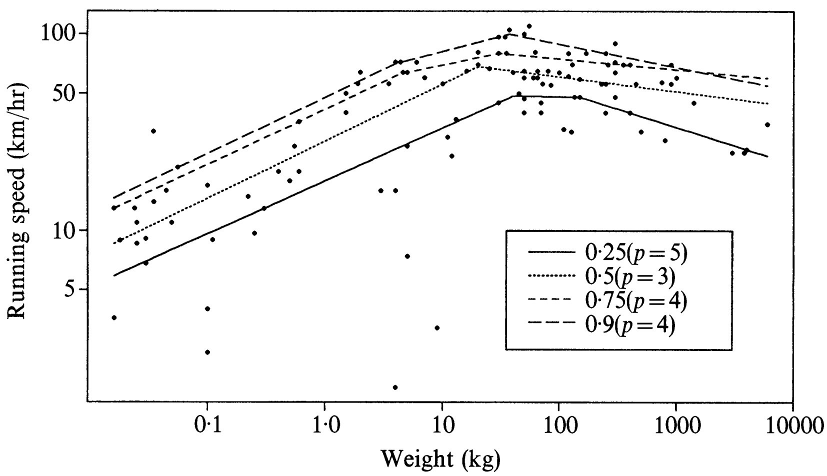

Fig. 3. Mammal data and four quantile L_1 smoothing splines.

ing that we have done none of the preliminary data editing which seems essential to the success of the least squares based methods. The simple piecewise linear form of the L_1 splines make them a natural technique for estimating linear change-point models. Friedman & Silverman (1989) present an alternative approach to fitting a piecewise linear regression spline using least squares methods.

In Fig. 3 we illustrate several distinct quantile smoothing splines for the same data. Here the upper quantiles are of particular interest since they represent the envelope of biological feasibility. In Fig. 3 we have again chosen λ for the median and 90th percentile by the Schwarz criterion; however, this produces a rather rough fit with $p_{\hat{\lambda}}=8$ for the 25th percentile and $p_{\hat{\lambda}}=7$ for the 75th. So we have selected somewhat larger λ's for these curves to achieve a more consistent degree of smoothness. Even so, the 75th and 90th percentile curves cross in Fig. 3 indicating, perhaps, that the 75th may still be somewhat oversmoothed, or simply that there are not enough data to distinguish these two quantiles for the larger animals.

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