Order-Preserving Nonparametric Regression, With Applications to Conditional Distribution and Quantile Function Estimation

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Short title. Order-Preserving Nonparametric Regression.

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Abstract

In some regression problems we observe a 'response' Y_{ti} to level t of a 'treatment' applied to an individual with level X_i of a given characteristic, where it has been established that response is monotone increasing in the level of the treatment. A related problem arises when estimating conditional distributions, where the raw data are typically independent and identically distributed pairs (X_i, Z_i) , and Y_{ti} denotes the proportion of Z_i 's that do not exceed t. We expect the regression means $g_t(x) = E(Y_{ti}|X_i = x)$ to enjoy the same order relation as the responses, i.e. $g_t \leq g_s$ whenever $s \leq t$. This requirement is necessary in order to obtain bona fide conditional distribution functions, for example. If we estimate g_t by passing a linear smoother through each data set $\mathcal{X}_t = \{(X_i, Y_{ti}) : 1 \leq i \leq n\}$ then the order-preserving property is guaranteed if and only if the smoother has nonnegative weights. However, in such cases the estimators generally have high levels of boundary bias. On the other hand, the order-preserving property usually fails for linear estimators with low boundary bias, such as local linear estimators, or kernel estimators employing boundary kernels. This failure is generally most serious at boundaries of the distribution of the explanatory variables, and ironically it is often in just those places that estimation is of greatest interest, since responses there imply constraints on the larger population. In this paper we suggest nonlinear, order-invariant estimators for nonparametric regression, and discuss their properties. The resulting estimators are applied to the estimation of conditional distribution functions at endpoints and also change-points. The availability of bona fide distribution function estimators at endpoints also enables the computation of change-point diagnostics that are based on differences in a suitable norm between two estimated conditional distribution functions, obtained from data that fall into one-sided bins.

Key words: Bias reduction, boundary effect, change-point, endpoint, linear methods, local linear estimator, monotonicity, Nadaraya-Watson estimator, prediction.

1. Introduction

1.1. Regression problems requiring order-preserving solutions. Suppose we observe a 'response,' Y_{ti} , to level t of a 'treatment' applied to an individual with level X_i of a given characteristic, where it has been established that response is monotone across the range of the treatment. For instance, Y_{ti} might represent the height at age t years of the ith child in a growth study, where the child's mother's height was X_i units. We expect the regression means, $E(Y_{ti}|X_i=x)$, to be monotone in t for fixed x, but monotonicity of the estimators is not assured by conventional nonparametric regression smoothers. Difficulties with monotonicity can be particularly acute towards the ends of the design interval. In many applications it is on just those places that the majority of interest centers.

A major motivating example to consider in this setting is the nonparametric estimation of a conditional distribution function. This problem is of interest in its own right, but also has applications to the estimation of conditional density functions and quantile functions which usually are derived from a suitable conditional distribution function estimate. Suppose we observe a sequence of independent and identically distributed data pairs (X_i, Z_i) , for $1 \le i \le n$, and wish to construct an estimator $\widehat{F}(\cdot|x)$ of the conditional distribution function $F(t|x) \equiv P(Z \le t|X = x)$. This problem admits a simple solution in terms of nonparametric regression, since if we define $Y_{ti} = I(Z_i \le t)$ then F(t|x) equals the mean of Y_{ti} given $X_i = x$. We would of course require $\widehat{F}(t|x)$ to be a bona fide distribution function estimate, i.e., to be monotone increasing in t, but this property is not guaranteed by passing conventional regression smoothers through the data set $\mathcal{X}_t = \{(X_i, Y_{ti}) : 1 \le i \le n\}$.

Estimating a conditional distribution function at a boundary or endpoint of the support of the covariates is of special interest, for two reasons. First, we may wish to construct prediction intervals for a new observation that will be made right at the boundary of the current domain of the covariate, as is often the case when observations are made sequentially involving regular small increments of the covariate, such as in quality control or environmental applications. Such prediction intervals are conveniently based on estimated conditional distributions. Secondly, for the detection and estimation of change-points that may involve changes in features of the conditional distribution that are more general than just mean changes, the estimation of bona fide conditional distribution functions at endpoints will provide an essential tool. Differences in a suitable metric between estimated left- and right-sided conditional distribution functions, based on one-sided windows placed around an assumed change-point location, and taken as a function of this assumed location, provide change-point diagnostics.

The present paper addresses this problem by introducing the more general perspective of order-preserving nonparametric regression. Specifically, we address sequences of data sets $\mathcal{X}_t = \{(X_i, Y_{ti}) : 1 \leq i \leq n\}$, for $t \in \mathcal{T}$, where the explanatory variables X_i are common to each \mathcal{X}_t , and \mathcal{T} denotes an interval which might be either bounded or unbounded, either discrete or in the continuum. The pairs (X_i, Y_{ti}) may often be regarded as observations of a generic (X, Y_t) , say. The Y_{ti} 's are ordered, in the sense that for each $i, Y_{si} \leq Y_{ti}$ whenever $s \leq t$. Therefore, we expect the regression means $g_t(x) = E(Y_t|X=x)$ to be ordered: $g_s(x) \leq g_t(x)$ whenever $s \leq t$ and x is in the support interval \mathcal{I} of the distribution of X. We wish to construct a sequence of estimators $\{\hat{g}_t : t \in \mathcal{T}\}$, of the set of functions $\{g_t : t \in \mathcal{T}\}$, which enjoys the same ordering property. If it does, then we say the estimators are order-preserving on \mathcal{I} . We shall suggest order-preserving regression smoothers with relatively low bias, particularly at the extremities of the design interval, and describe their properties.

1.2. Existing order-preserving methods. Quotient methods for nonparametric regression, for example the Nadaraya-Watson estimator, are order-preserving, if based on non-negative kernel weights. This follows from the fact that such techniques (a) are linear in the response variables Y_i , and (b) have the positivity property, i.e., whenever the response variables are all nonnegative, the estimator itself is nonnegative. More generally, a linear estimator is order-preserving if and only if it has the positivity property.

Several recent examples of quotient methods are based on the Nadaraya-Watson estimator. They include identity-reproducing regression or mass-centered smoothing techniques, discussed by Müller and Song (1993) and Mammen and Marron (1997); the biased bootstrap form of the Nadaraya-Watson estimator (Hall and Presnell, 1988); and some, although not all, data-sharpening techniques (Choi, Hall and Rousson, 1999). However, all these methods suffer excessive bias at boundaries. Specifically, while they have $O(h^2)$ bias in the interior, where h denotes bandwidth, this rate deteriorates to O(h) near a boundary.

Convolution-type estimators, such as those of Gasser-Müller and Priestley-Chao type (see, e.g., Wand and Jones, 1995, p. 130ff; Simonoff, 1996, p. 138), are also order-preserving, as long as positive kernel weights are used, since they are linear and have the positivity property. For both convolution-type and quotient-type estimators, the positivity property holds if the kernels used are non-negative. On the other hand, local-linear methods, which are well known for their high level of resistance to boundary effects (see e.g. Fan, 1992, and Fan and Gijbels, 1992), lack the positivity property and are not order preserving, even while employing a non-negative

kernel or weight function. Moreover, they suffer this deficiency even in the asymptotic limit — in an important class of problems the probability that a local-linear estimator, computed for a particular realization, is not order preserving at the boundary, converges to 1 as sample size increases; see section 3.1.

In fact, no linear, kernel-type estimator which enjoys the positivity property can have better than O(h) bias at the boundary, where h denotes the estimator's bandwidth; see section 3.1. Equivalently, no order-preserving kernel-type estimator with better than O(h) boundary bias can be linear. Therefore, nonlinear estimators must be used if we are to obtain an order-preserving estimator with $O(h^2)$ bias across the full design interval. In particular, none of the estimators discussed above is suitable. This also includes traditional methods for alleviating edge effect problems based on boundary kernels, as it can be easily shown that suitable boundary kernel functions cannot be restricted to be non-negative.

1.3 The relevance of conditional distribution function estimation at boundaries. As mentioned above, a major motivation for order-preserving regression is the desire to obtain bona fide distribution function estimates (see, for example, Hall et al., 1999, and Peracchi, 2002, for some recent work on this problem). Such estimates are important for a variety of purposes, of which one is estimation of conditional density functions which are implicitly derived via conditional distribution functions. Another application is the nonparametric estimation of conditional quantile functions as inverses of conditional distribution functions, a problem that has been studied by Bhattacharya and Gangopadhyay (1990) and Yu and Jones (1998), among others. There is particular motivation for estimating bona fide conditional distribution functions exactly at those covariate levels where the problem is hardest, namely at or near endpoints and change-points defined in terms of the covariate level.

2. Methodology

While it is clear from discussion in section 1 that order-preserving methods with good boundary-bias properties are necessarily nonlinear, the linearity of techniques such as those of Nadaraya and Watson, Gasser and Müller, and Priestley and Chao is partly responsible for their order-preserving property. Therefore, we seek a method which combines the best of both worlds, i.e., which corrects for boundary bias without losing the important features of linearity. This leads us to suggest that nonlinear methods be used to impute ordered 'pseudo-data' on the sides

of boundaries away from the real data set, and that then relatively conventional linear methods be applied to the new, larger data set, to produce an estimator which is order-preserving.

Data imputation by reflection in the boundaries, much as discussed by Schuster (1985), Silverman (1986, p. 30f) and Cline and Hart (1991) in the context of density estimation, leads directly to an order-preserving estimator. It enjoys only O(h) bias at the boundaries, however. Hall and Wehrly (1991) suggested an alternative data imputation method which involves reflection in points on the boundaries, but while it has good boundary bias properties it fails to be order-preserving. We propose an order-preserving version of the Hall-Wehrly technique, which attains the desirable $O(h^2)$ boundary bias rate, as follows.

Assume we have an ordered sequence of data sets \mathcal{X}_t , as suggested in section 1.1; in particular, $Y_{si} \leq Y_{ti}$ whenever $s \leq t$. Suppose the distribution of the explanatory variables X_i is supported on an interval $\mathcal{I} = [a, b]$, which we call the design interval. Let $\hat{g}_{\text{LL},t}$, for $t \in \mathcal{T}$, denote a local linear estimator of g_t computed from data in \mathcal{X}_t . It is defined by minimizing the weighted sum of squares

$$\sum_{i=1}^{n} K\left(\frac{x - X_i}{h}\right) [Y_{ti} - \{\beta_0 + \beta_1(x - X_i)\}]^2$$

with respect to β_0 , β_1 and setting $\hat{g}_{LL,t} = \hat{\beta}_0$. Here K is a kernel function and h the sequence of bandwidths.

For x = a or x = b consider the sequence $\mathcal{U}(x) = \{\hat{g}_{\mathrm{LL},t}(x) : t \in \mathcal{T}\}$. Ideally the elements of each $\mathcal{U}(x)$ would be monotone increasing in t, but this is unlikely to be the case for the endpoints x = a, b. We wish to 'monotonize' $\hat{g}_{\mathrm{LL},t}(x)$ at just those places. There are several ways of achieving this end; we consider one particular method below, where we denote the monotonized version of $\hat{g}_{\mathrm{LL},t}(x)$ (monotone in the sense of a function of t, for fixed x) by $\tilde{g}_t(x)$. In effect it fills in the valleys of $\hat{g}_{\mathrm{LL},t}(x)$ by horizontal lines. For the special case of estimating a conditional distribution function, this is indicated in Figure 1 for an example data set. The initial non-monotone (in t) estimate $\hat{F}_{\mathrm{LL}}(\cdot, x)$ of the conditional distribution function is monotonized to produce the version $\hat{F}(\cdot|x)$.

For simplicity we assume that \mathcal{T} is closed and bounded, although our methods lead to a more general definition of \tilde{g}_t . The prescription given below is descriptive, but can readily be given in mathematically rigorous terms. Let $\mathcal{V}(x)$ be the set of points t which are such that $\hat{g}_{\text{LL},u}(x) \leq \hat{g}_{\text{LL},t}(x)$ for all $u \leq t$, and also such that, on passing to a point in \mathcal{T} immediately to the right of t, $\hat{g}_{\text{LL},t}(x)$ turns strictly downwards, rather than taking a nondecreasing path.

In practical applications $\mathcal{V}(x)$ would be finite, so we write it in strictly increasing order as $\mathcal{V}(x) = \{s_1, \ldots, s_N\}$. For each $s \in \mathcal{V}$, let u(s) be the point $t \in \mathcal{T}$ at which $\hat{g}_{\text{LL},t}(x)$ first recovers the same level as, or a greater level than, $\hat{g}_{\text{LL},s}(x)$. Put $t_i = u(s_i)$ and define $\tilde{g}_t(x) = \hat{g}_{\text{LL},s_i}(x)$ if $s_i \leq t < t_i$ for some i, and $\tilde{g}_t(x) = \hat{g}_{\text{LL},t}(x)$ otherwise. (Definitions near the boundary are handled in the obvious way; see Figure 1.) Then $\tilde{g}_t(x)$ is nondecreasing in $t \in \mathcal{T}$.

For each $t \in \mathcal{T}$, we then compute pseudo-data by projecting the points in \mathcal{X}_t through both $\tilde{g}_t(a)$ and $\tilde{g}_t(b)$; see Figure 2 for the distribution function case. This produces a new data set $\mathcal{X}'_t = \{(X'_i, Y'_{ti}) : 1 \leq i \leq 3n\}$, say, where without loss of generality, $X_1 \leq \ldots \leq X_{3n}$. Thus, the middle n pairs (X'_i, Y'_{ti}) are the original data, the first n are pseudo-data on the left-hand side of the lower boundary, and the last n are pseudo-data on the right-hand side of the upper boundary.

We compute \hat{g}_t by fitting a kernel-type linear estimator through \mathcal{X}'_t , assuming that the estimator has the form

$$\hat{g}_t(x) = \sum_{i=1}^{3n} w_i(x) Y'_{ti}, \qquad (2.1)$$

where, for a constant C > 0, the weights satisfy:

for
$$1 \le i \le 3n$$
, $w_i(\cdot) \ge 0$ and $w_i(x) = 0$ whenever $|x - X_i'| > Ch$; (2.2)

for $1 \le i \le n$ and $0 \le x \le Ch$, $w_{n-i+1}(a+x) \le w_{n+i}(a+x)$

and
$$w_{2n-i+1}(b-x) \le w_{2n+i}(b-x)$$
. (2.3)

Condition (2.2) is of course satisfied by kernel-type estimators based on nonnegative kernels supported in the interval [-C, C]. Condition (2.3) is also typically satisfied. To appreciate why, observe that by definition of our reflection method, the set of design points of the pseudo-data generated on the left-hand side of a (respectively, on the right-hand side of b) is the reflection in x = a (respectively, in x = b) of the set of design points of the real data. When \hat{g}_t is a Nadaraya-Watson estimator, the choice we make in the illustrating examples, the weight $w_i(x)$ equals the ratio of a single kernel weight $K_i(x) = K\{(x - X_i)/h\}$ to the sum $\sum_j K_j(x)$. If K is symmetric, unimodal and supported on [-C, C] then, provided $h \leq (b - a)/(2C)$, this construction implies that at a + x, with $0 \leq x \leq Ch$, the denominators of $w_{n-i+1}(\cdot)$ and $w_{n+i}(\cdot)$ are identical, but (by virtue of the unimodality) the numerator of the latter is not less than that of the former. This property, and its counterpart for the other boundary, imply (2.3).

This last smoothing step, when implemented with a Nadaraya-Watson quotient type kernel estimator, is illustrated for the conditional distribution function case in Figure 3 for an example data set. The resulting distribution function estimator is denoted by $\widehat{F}(\cdot|x)$.

The following result, proved in section 3, demonstrates that \hat{g}_t has the required properties.

Theorem 2.1. If \hat{g}_t is defined by (2.1), if the weights satisfy (2.2) and (2.3), and if $0 < h \le \frac{1}{2}(b-a)$, then \hat{g}_t is order preserving on \mathcal{I} .

3. Theoretical Properties

3.1. Problems suffered by linear estimators. Let $\hat{g}(x) = \sum_i w_i(x) Y_i$ be a linear estimator of g(x) = E(Y|X = x), computed from the independent and identically distributed data $\mathcal{X} = \{(X_i, Y_i) : 1 \leq i \leq n\}$. We shall say that \hat{g} is of kernel type with bandwidth h if the w_i 's are functionals of X_1, \ldots, X_n satisfying, for constants $C_1, C_2, C_3 > 0$, for all x in the design interval, and for all sufficiently large n,

$$w_i(x) = 0$$
 whenever $|x - X_i| > C_1 h$, and $\sum_{i:|x - X_i| > C_2 h} w_i(x) \ge C_3$. (3.1)

Conventional kernel estimators, such as those of Nadaraya-Watson, Gasser-Müller or Priestley-Chao type, satisfy this condition with probability 1 when the kernel is nonnegative and compactly supported, when the design density is bounded away from 0 on the design interval, and when the bandwidth satisfies the mild conditions $h = h(n) \to 0$ and $nh/(\log n)^{1/2} \to \infty$.

Assume the design interval is [a, b]. Our first result shows, in effect, that no kernel-type linear estimator with the positivity property can have better than O(h) bias at the boundary. Since a linear estimator is order preserving if and only if it has the positivity property, then linear, order-preserving estimators fail to have good bias properties.

Theorem 3.1. If \hat{g} is a kernel-type linear estimator with the positivity property, and if in the case where $g(x) \equiv C$ (a constant) we have

$$E\{\hat{g}(a)|X_1,\dots,X_n\} = C + o_p(h)$$
(3.2)

as $h \to 0$, then whenever g has a continuous derivative on [a,b] and $g'(a) \neq 0$, there exists $\epsilon > 0$ such that the probability that

$$|E\{\hat{g}(a)|X_1,\ldots,X_n\}-g(a)|>\epsilon h$$

converges to 1 as $n \to \infty$.

In general, local linear estimators fail to have the positivity property, although it might be thought that this is only a rare defect — for large samples, local linear estimators of regression means might be expected to be order-preserving except in unusual cases. Unfortunately this is not true. Below we shall show that with probability tending to 1, local linear methods fail to be order preserving in the important case of distribution function estimation. This is only one member of a large class of examples for which local linear methods fail to be order-preserving.

The problems arise because of the way local linear methods deal with edge effects. On the other hand, if the design density is supported on a compact interval \mathcal{I} and bounded away from 0 there, then with probability tending to 1 as $n \to \infty$, local linear estimators have the positivity property when applied to data pairs whose design component is confined to a compact subinterval of \mathcal{I} which does not include the endpoints of \mathcal{I} . Therefore, local linear estimators seldom fail to be order preserving in the interior of \mathcal{I} . We compile some assumptions as follows.

C0 Let (X_i, Z_i) , for $1 \le i \le n$, be a sequence of independent and identically distributed random 2-vectors, with the marginal distribution of X being supported on an interval $\mathcal{I} = [a, b]$, and the marginal density continuous and non-vanishing there. Construct an estimator $\widehat{F}_{LL}(t|x)$ of $F(t|x) = P(Z \le t|X = x)$ by passing a local linear smoother through the pairs (X_i, Y_{ti}) , where $Y_{ti} = I(Z_i \le t)$, using a bounded, compactly supported, symmetric, piecewise continuous, nonnegative kernel K and a bandwidth h. Assume that $h = h(n) \to 0$ and $h \to \infty$ as $h \to \infty$, which are minimum conditions for weak consistency. We also ask that for x = a and h, $F(\cdot|x)$ be nonsingular.

Theorem 3.2. Under conditions (C0), and with probability tending to 1 as $n \to \infty$, there exist intervals $[a, \hat{x}_1]$ and $[\hat{x}_2, b]$, with \hat{x}_1, \hat{x}_2 stochastic and $a < \hat{x}_1 < \hat{x}_2 < b$, such that whenever x is an element of either interval, $\widehat{F}_{LL}(\cdot|x)$ is not monotone nondecreasing.

It may be proved, under slightly more restrictive conditions, that the lengths of the intervals $[a, \hat{x}_1]$ and $[\hat{x}_2, b]$ are both $O_p(h)$, and that they may be chosen so that with probability tending to 1 their lengths exceed ϵh , provided $\epsilon > 0$ is taken sufficiently small (but fixed). Furthermore, the problems evinced by Theorem 3.2 are not overcome by modifying local linear estimators in conventional ways. For example, incorporating a ridge parameter does not alleviate the

difficulties, since it alters only the denominators of the smoothing weights used to construct local linear estimators; the non-positivity of local linear methods, which is the root cause of the problems, is caused by the numerators of the smoothing weights.

3.2. Properties of the order-preserving estimator \hat{g}_t . For the sake of definiteness we shall take \hat{g}_t , defined in section 2 and computed from the data and pseudo-data, to be a standard Nadaraya-Watson estimator, although our results apply to other estimator types as well. The Nadaraya-Watson kernel estimator for $g_t(x)$, obtained from the pseudo-data (X'_i, Y'_{ti}) , is

$$\hat{g}_t(x) = \sum_{i=1}^{3n} K\left(\frac{x - X_i'}{h}\right) Y_{ti}' / \sum_{i=1}^{3n} K\left(\frac{x - X_i'}{h}\right).$$

With the aim of obtaining useful upper bounds, we compile the following assumptions:

C1 For each t the 2-vectors (X_i, Y_{ti}) , for $1 \leq i < \infty$, are independent and identically distributed; the common distribution of the independent random variables X_i is continuous on a compact interval \mathcal{I} , has a density which is bounded away from 0 and has two bounded derivatives there, and vanishes off \mathcal{I} ; for some $\epsilon > 0$,

$$\sup_{t \in \mathcal{T}, |u| < \epsilon} E\left(\exp\left[u\{Y_{ti} - E(Y_{ti}|X_i)\}\right]\right) < \infty; \tag{3.3}$$

the regression-mean functions $g_t(x) = E(Y_{ti}|X_i = x)$, for $t \in \mathcal{T}$, and their first two derivatives, are bounded uniformly with respect to both $x \in \mathcal{I}$ and $t \in \mathcal{T}$; the bandwidths h_1 used to construct the local linear estimator $\hat{g}_{\text{LL},t}$ from the data set \mathcal{X}_t , and h_2 used to construct the Nadaraya-Watson estimator \hat{g}_t from \mathcal{X}'_t , both satisfy $n^{\epsilon}h_j \to 0$ and $n^{1-\epsilon}h_j \to \infty$ as $n \to \infty$ for some $\epsilon > 0$; the kernels used for either estimator are symmetric, compactly supported, nonnegative, and Hölder continuous on the real line; the kernel used for \hat{g}_t is unimodal; and the number of elements of $\mathcal{T} = \mathcal{T}(n)$ increases no more than polynomially fast in n.

Theorem 3.3. Assume conditions (C1). Then with probability 1,

$$\sup_{t \in \mathcal{T}} \sup_{x \in \mathcal{X}} |\hat{g}_t(x) - g_t(x)| = O\{(nh)^{-1/2} (\log n)^{1/2} + h^2\}.$$
 (3.4)

The rate of convergence asserted at (3.4) is the best possible for even a single t, and for distributions satisfying (C1). In fact, it may be proved that in the case of a single regression, and under additional regularity conditions,

$$\sup_{x \in \mathcal{X}} |\hat{g}_t(x) - E\{\hat{g}_t(x)|X_1, \dots, X_n\}| = C\{1 + o(1)\} (nh)^{-1/2} (\log n)^{1/2}$$

with probability 1, where C > 0 is a constant; and $E\{\hat{g}_t(x)|X_1,\ldots,X_n\} = h^2\gamma_t(x) + o(h^2)$ with probability 1, where γ_t is a non-vanishing function. Therefore, the convergence rate at (3.4) is also best possible when it is asserted uniformly in t. We note that the final assumption in condition (C1), about the rate at which the number of elements (size) of $\mathcal{T}(n)$ increases, is usually adequate even when \mathcal{T} is infinite, and also that there is no difficulty extending our methods and results to the fixed design case where X_1, \ldots, X_n are non-stochastic and spaced according to a smooth positive design density.

3.3. Application to Distribution Function Estimation. Depending on the model that generates the ordered data sets \mathcal{X}_t , alternative methods can be used to derive rates of convergence of \hat{g}_t to g_t in integral metrics, not requiring the logarithmic factor on the right-hand side of (3.4). For instance, this is the case for the distribution function estimation problem.

In that context we observe independent and identically distributed data pairs $(X_1, Z_1), \ldots$, (X_n, Z_n) ; we put $Y_{ti} = I(Z_i \leq t)$ and $F(t|x) = P(Z \leq t|X = x)$, and we take $\widehat{F}(t|x)$ to be the estimator obtained by applying our order-preserving smoother to the data sets $\mathcal{X}_t = \{(X_i, Y_{ti}) : 1 \leq i \leq n\}$, for $t \in (-\infty, \infty)$. Consider the following assumptions.

C2 The distribution of (X, Z) is compactly supported; the distribution of X is continuous on a compact interval \mathcal{I} , has a density which is bounded away from 0 and has two bounded derivatives there, and vanishes off \mathcal{I} ; the functions $(\partial/\partial t)^j F(t|x)$, for j=0,1,2, are bounded uniformly with respect to both $x \in \mathcal{I}$ and $t \in \mathcal{T}$; the bandwidths h_1 used to construct the local linear estimator $\hat{g}_{\text{LL},t}$ from the data set \mathcal{X}_t , and h_2 used to construct the Nadaraya-Watson estimator \hat{g}_t from \mathcal{X}'_t , both satisfy $n^{\epsilon}h_j \to 0$ and $n^{1-\epsilon}h_j \to \infty$ as $n \to \infty$ for some $\epsilon > 0$; the kernels used for either estimator are symmetric, compactly supported, nonnegative, and Hölder continuous on the real line; and the kernel used for \hat{g}_t is unimodal.

Theorem 3.4. Assume conditions (C2). Then, with probability 1,

$$\int \int \left\{ \widehat{F}(t|x) - F(t|x) \right\}^2 dt \, dx = O\left\{ (nh)^{-1} + h^4 \right\}.$$

Theorem 3.4 implies a uniform convergence rate for estimators of linear functionals of $F(t|\cdot)$. For example, given a constant B>0, let $\mathcal{C}(B)$ denote the class of differentiable functions ψ satisfying $\sup_t |\psi'(t)| \leq B$, and define $\Psi(x|\psi) = E\{\psi(Z)|X=x\}$. Put $\widehat{\Psi}(x|\psi) = \int \psi(t) \, d_t \widehat{F}(t|x)$. Applying Theorem 3.4 through an integration by parts and an application of Hölder's inequality, we obtain that with probability 1,

$$\sup_{\psi \in \mathcal{C}(B)} \int \left\{ \widehat{\Psi}(x|\psi) - \Psi(x|\psi) \right\}^2 dx = O\left\{ (nh)^{-1} + h^4 \right\}.$$

Another case of interest concerns the estimation of conditional quantiles. Assume that for $0 \le q < r \le 1$ the inverse $F^{-1}(p|x)$ of $F(\cdot|x)$ exists for $p \in [q,r]$, furthermore that $\inf_{p \in [q,r]} \inf_{x \in \mathcal{X}} F'(F^{-1}(p))|x) > 0$. Then, choosing for example as estimates of conditional quantiles

$$\hat{F}^{-1}(p|x) = \frac{1}{2} \left[\inf_{t \in \mathcal{T}} \{ t : \hat{F}(t|x) \ge p \} + \sup_{t \in \mathcal{T}} \{ t : \hat{F}(t|x)$$

the result (3.4), applied to conditional distribution functions and combined with bounds for the difference of inverses of two functions, leads to: with probability 1,

$$\sup_{p \in [q,r]} \sup_{x \in \mathcal{X}} |\hat{F}^{-1}(p|x) - F^{-1}(p|x)| = O\{(nh)^{-1/2}(\log n)^{1/2} + h^2\}.$$

4. Illustrations of order-preserving nonparametric regression

We demonstrate here some simulation and application based examples that focus on the case of conditional distribution estimation. Applying the three-step order-preserving nonparametric regression procedure described in section 2, to data $(X_i, Y_{ti}) = (X_i, I(Z_i \leq t))$, for i = 1, ..., n, we first obtain the augmented pseudo-data, (X'_i, Y'_{ti}) , for i = 1, ..., 3n, and then the bona fide conditional distribution function estimator

$$\widehat{F}(t|x) = \frac{\sum_{i=1}^{3n} K\left(\frac{x - X_i'}{h}\right) Y_{ti}'}{\sum_{i=1}^{3n} K\left(\frac{x - X_i'}{h}\right)}.$$
(4.1)

In the following, we choose the kernel function K to be the Bartlett-Parzen-Epanechnikov kernel with support [-1,1], $K(u) = \frac{3}{4}(1-u^2)I(-1 \le u \le 1)$. The transition from the initial

non-monotone conditional distribution function estimator $\hat{F}_{LL}(\cdot|b)$ to the monotonized version $\tilde{F}(t|b)$ is illustrated in Figure 1. Generation of the pseudo-data and the final estimate (4.1) is depicted in Figures 2 and 3. If one desires an estimate of the conditional distribution function that is smooth in t, one could use (4.1) as a starting point and then integrate the conditional density kernel estimator $\hat{f}(t|x) = \int \tilde{h}^{-1} \tilde{K}(\tilde{h}^{-1}(t-u)) d\hat{F}(u|x)$ (constructed with kernel \tilde{K} and bandwidth \tilde{h}) to obtain the smooth estimate $\tilde{F}(t|x) = \int_{-\infty}^{t} \hat{f}(v|x) dv$. The preceding formula demonstrates that nonparametric estimation of a conditional density requires a bona fide non-negative conditional empirical measure, which is only guaranteed if an order-preserving procedure is used.

4.1. Application to Change-Point Estimation and Conditional Distribution Estimation Near Change-Points. We illustrate the use of conditional distribution and quantile function estimation near and at endpoints, through an application to the estimation of change-point locations and of conditional distribution and quantile functions near change-points. We consider here a small number of isolated change-point locations θ , at which the map from the domain of the covariate [a, b] to the space of distribution functions, $x \mapsto F(\cdot|x)$, has a discontinuity, whereas at all other covariate values x it is continuous. Continuity is defined with respect to a suitable metric in the space of distribution functions (Carlstein, 1988).

Consider a covariate level x_0 in the interior of [a, b], and denote the conditional distributions (pertaining to the L^2 -metric) to the left and right of x_0 as $F_-(\cdot|x_0) = \lim_{x \uparrow x_0} F(\cdot|x)$ and $F_+(\cdot|x_0) = \lim_{x \downarrow x_0} F(\cdot|x)$, respectively. With $D(F_-(\cdot|x_0), F_+(\cdot|x_0)) = \int \{F_+(t|x_0) - F_-(t|x_0)\}^2 dt$, one has $D(F_-(\cdot|x_0), F_+(\cdot|x_0)) = 0$ if the mapping $x \mapsto F(\cdot|x)$ is continuous at $x = x_0$, and $D(F_-(\cdot|x_0), F_+(\cdot|x_0)) > 0$ if a jump occurs at x_0 .

We may estimate $F_{\pm}(\cdot|x_0)$ using the order-preserving estimators $\widehat{F}_{\pm}(\cdot|x_0)$, by using only the data falling into $[a, x_0]$ when computing $\widehat{F}_{-}(\cdot|x_0)$, with reflection occurring at the endpoints a and x_0 ; and analogously for $\widehat{F}_{+}(\cdot|x_0)$. In both cases, x_0 plays the role of an endpoint.

Using the change-point detection function $\Delta(\theta) = \int \left\{ \widehat{F}_+(t|\theta) - \widehat{F}_-(t|\theta) \right\}^2 dt$, the corresponding change-point location estimate is $\hat{\theta} = \arg\sup_{\theta} \Delta(\theta)$. If more than one change-point is to be estimated, this process is simply repeated, by removing the previously estimated locations plus appropriate neighborhoods around them from the set of potential change-point locations over which a maximum of $\Delta(\cdot)$ is sought.

Once the estimated change-point location $\hat{\theta}$ has been determined, we set $x_0 = \hat{\theta}$ and obtain order-preserving distribution function estimates using only data where the covariate values fall

into the intervals $[a, \hat{\theta}]$ on the left of the estimated change-point, or into the intervals $[\hat{\theta}, b]$ on the right of the estimated change-point, following exactly the same procedures as for an assumed change-point at x_0 .

4.2. Simulated Example for Change in Variance. We illustrate these procedures first with a simulated data set. Here

$$Z_i = g(X_i) + e_i, i = 1, \dots, n, \quad X_i \sim U(0, 1), \quad e_i \sim N(0, \sigma^2),$$

and the e_i 's and X_i 's are totally independent. Choosing n=1000, we assume that a change in the variance occurs at x=0.7, with $g(x)=e^x$ and $var(e|x)=\sigma^2=0.2$, x<0.7, while $var(e|x)=\sigma^2=1$, x>0.7. The bandwidth was chosen as h=0.2.

We obtain the change-point detection function $\Delta(\cdot)$ as shown in Figure 4. A single change-point location emerges as the maximizing argument, and the conditional distribution function estimates adapted to this estimated change-point location are indicated by the 0.1, 0.5 and 0.9 estimated quantiles in Figure 5. The change in variance is very clearly reflected in these estimates. Figure 6 allows comparison of the two conditional distribution function estimates $\widehat{F}_{-}(\cdot|\widehat{\theta})$ and $\widehat{F}_{+}(\cdot|\widehat{\theta})$ right at the endpoint $\widehat{\theta}$, with the corresponding normal underlying distribution functions $F_{-}(\cdot|\theta)$ and $F_{+}(\cdot|\theta)$. Agreement is seen to be quite good, confirming that order-preserving estimation of conditional distribution functions performs well at both change-points and endpoints.

Note that the characteristic of the distribution function that is subject to a sudden change is unknown, i.e., it is not assumed to be known in this example that it is a jump in the variance. Commonly used change-point detection methods based on differences between regular one-sided local linear fits are focusing on mean changes and will not detect this change, since the mean continues to change smoothly across the point of discontinuity in the variance. One-sided bona fide distribution function estimates at endpoints then allow to define a general detection function Δ based on a suitable distance measure between left- and right-sided distribution function estimates.

4.3. Application to Change-Points in DNA Sequences. The analysis of the frequencies of base-pairs in DNA sequences has been studied by many authors; see for example Braun and Müller (1999), Braun et al. (2000), Chechetkin and Lobzin (1998) and Liö et al. (1996) for biological relevance, methodology and further references. We use the sequence of Saccharomyces

Cerevisiae III, a chromosome of brewer's yeast, to illustrate order-preserving conditional distribution function estimation in the presence of change-points.

The data consist of n = 526 relative frequencies (obtained by binning) of the occurrence of Guanine and Cytosine (G+C) as a proportion of all bases (A,C,G and T). These data are available from Genbank (http://www.ncbi.nlm.nih.gov/Genbank/). We assume two change-points, based on previous analyses of these data. One could extend existing inference procedures as in Dümbegn (1991) or Braun et al. (2000) for the existence and number of change-points to the more complex situation in this application. Our analysis proceeds by first locating the change-points with the methods described above and then constructing the order-preserving conditional distribution function estimates, adapted to the two estimated change-points as shown via the quantile estimates in Figure 7. Interesting mean and variance patterns become visible that may motivate further, detailed analyses.

5. Theoretical arguments

5.1. Proof of Theorem 2.1. Recall that $\mathcal{X}'_t = \{(X'_i, Y'_{ti}) : 1 \leq i \leq 3n\}$, where $X_1 \leq \ldots \leq X_{3n}$. We must establish that if $s \leq t$ then, for $x \in \mathcal{I}$ and $h \leq \frac{1}{2}(b-a)$,

$$\hat{g}_t(x) - \hat{g}_s(x) = \sum_{i=1}^{3n} w_i(x) \left(Y'_{ti} - Y'_{si} \right) \ge 0.$$
 (5.1)

If $n+1 \le i \le 2n$ then (X_i', Y_{ti}') is one of the original data, and so by assumption (see section 2), $Y_{ti}' - Y_{si}' \ge 0$, implying that the corresponding contribution to the series in (5.1) is nonnegative. If $1 \le i \le n$ then either $Y_{ti}' - Y_{si}' \ge 0$, in which case the contribution to (5.1) is nonnegative, or $Y_{ti}' - Y_{si}' < 0$. In the latter case, the manner of generation of the pseudo-data implies that there exists an index j, between n+1 and 2n, such that X_j' is the same distance to the right of x=a as X_i' is to the left. Since $\tilde{g}_u(a)$ is nondecreasing as a function of u then $|Y_{ti}' - Y_{si}'| \le Y_{tj}' - Y_{sj}'$. In view of (2.3), $w_i(x) \le w_j(x)$, and so the net contribution of the ith and jth terms to the series in (5.1) is nonnegative. The case $2n+1 \le i \le 3n$ may be treated similarly. The assumption that $h \le \frac{1}{2}(b-a)$ implies that no real data pair needs to be combined in this manner with more than one pseudo-data pair. Hence, for each negative summand in the series in (5.1) there is a positive summand which is not less than the absolute value of the negative summand; and no positive summand has to be combined with two or more negative summands in this way. This establishes the inequality at (5.1).

5.2. Proof of Theorem 3.1. Property (3.2) implies that $\sum_i w_i(a) = 1 + o_p(h)$. Recall that positivity means $\hat{g}(x) \geq 0$ whenever each $Y_i \geq 0$, and so implies that each $w_i(x) \geq 0$. From these results, Taylor expansion, and both parts of (3.1), we may prove that, when $g'(a) \geq 0$,

$$E\{\hat{g}(a)|X_1, \dots, X_n\} = \sum_{i=1}^n w_i(a) g(X_i) = \sum_{i=1}^n w_i(a) \{g(a) + (X_i - a) g'(a)\} + o_p(h)$$

$$= g(a) + g'(a) \sum_{i=1}^n w_i(a) (X_i - a) + o_p(h)$$

$$\geq g(a) + g'(a) \sum_{i:|X_i - a| \geq C_2 h} w_i(a) (X_i - a) + o_p(h)$$

$$\geq g(a) + C_2 C_3 h g'(a) + o_p(h)$$

which implies the theorem. The case g'(a) < 0 may be treated similarly.

5.3. Proof of Theorem 3.2. Without loss of generality the design interval is [0, b]. We shall prove that with probability tending to 1, there exist s < t such that $\widehat{F}(t|0) - \widehat{F}(s|0) < 0$. This result, the continuity of $\widehat{F}(t|x)$ as a function of x, and the symmetry of behavior at either end of [0, b], imply Theorem 3.2.

Note first that it is possible to choose $\xi > 0$ such that $K(\xi) > 0$ and

$$A(\xi) \equiv \int_0^\infty y^2 K(y) \, dy - \xi \int_0^\infty y K(y) \, dy < 0.$$

Let $\delta > 0$ be so small that $K \geq C > 0$ on the interval $[\xi, \xi + \delta]$. Since $nh \to \infty$ then with probability tending to 1 as $n \to \infty$, there is at least one $X_i \in [\xi h, (\xi + \delta)h]$. Since $F(\cdot|0)$ is nonsingular then for this i we may choose s < t such that $Z_i \in (s, t)$ and no other Z_j lies there. (We suppress the dependence of s and t on i.) Then,

$$\widehat{F}(t|0) - \widehat{F}(s|0) = \frac{S_2 - (X_i/h) S_1}{S_2 S_0 - S_1^2} K\left(\frac{X_i}{h}\right),$$

where $S_k = (nh)^{-1} \sum_i (X_i/h)^k K(X_i/h)$. Now, $S_2 - (X_i/h) S_1 = A(X_i/h) f(0) + o_p(1)$, and as $n \to \infty$, $S_2 S_0 - S_1^2$ converges in probability to

$$f(0)^{2} \left[\frac{1}{2} \int_{0}^{\infty} y^{2} K(y) dy - \left\{ \int_{0}^{\infty} y K(y) dy \right\}^{2} \right] > 0,$$

where f denotes the marginal density of X. Hence, in view of our choice of X_i , the probability that $\widehat{F}(t|0) - \widehat{F}(s|0) < 0$ converges to 1 as $n \to \infty$, as had to be shown.

5.4. Outline proof of Theorem 3.3. Define $\mu_{\text{LL},t}(x) = E\{\hat{g}_{\text{LL},t}(x)|X_1,\ldots,X_n\}$. Using methods based on moderate deviations of sums of independent random variables, and in particular employing the assumption (3.3) of finite moment generating function, we may show that there exist $C_1, C_2 > 0$ such that, for all sufficiently large $C_3 > 0$,

$$\sup_{t \in \mathcal{T}} \max_{x=a,b} P\{ |\hat{g}_{LL,t}(x) - \mu_{LL,t}(x)| > C_3 (nh)^{-1/2} (\log n)^{1/2} \} = O(n^{-C_1 C_3}),$$

$$\sup_{t \in \mathcal{T}} \max_{x=a,b} P\{ |\mu_{LL,t}(x) - g_t(x)| > C_2 h^2 \} = O(n^{-C_3}). \tag{5.2}$$

From these results, the fact that \mathcal{T} has only $O(n^{C_4})$ elements for some $C_4 > 0$, and the Borel-Cantelli lemma, we may prove that with probability 1,

$$\sup_{t \in \mathcal{T}} \max_{x=a,b} |\hat{g}_{\mathrm{LL},t}(x) - g_t(x)| = O\{(nh)^{-1/2} (\log n)^{1/2} + h^2\}.$$

The latter property and the definition of \tilde{g}_t imply that, with

$$\xi_t(x) = \tilde{q}_t(x) \quad \text{and} \quad \eta = (nh)^{-1/2} (\log n)^{1/2} + h^2,$$
 (5.3)

we have with probability 1,

$$\sup_{t \in \mathcal{T}} \max_{x=a,b} \left| \xi_t(x) - g_t(x) \right| = O(\eta). \tag{5.4}$$

Assume the kernel used to construct the Nadaraya-Watson estimator \hat{g}_t is supported on [-C, C]. Then, \hat{g}_t restricted to [a+Ch, b-Ch] does not involve any of the pseudo-data. Define $\mu_t(x) = E\{\hat{g}_t(x)|X_1,\ldots,X_n\}$. Using the arguments leading to (5.2) we may prove that for constants $C_1, C_2 > 0$ we have for all sufficiently large $C_3 > 0$,

$$\sup_{t \in \mathcal{T}} \sup_{a+Ch \le x \le b-Ch} P\{ |\hat{g}_t(x) - \mu_t(x)| > C_3 (nh)^{-1/2} (\log n)^{1/2} \} = O(n^{-C_1 C_3}),$$

$$\sup_{t \in \mathcal{T}} \max_{x=a,b} P\{ |\mu_t(x) - g_t(x)| > C_2 h^2 \} = O(n^{-C_3}).$$

From this result, the fact that the kernel used to construct \hat{g}_t is Hölder continuous, the property that \mathcal{T} has only polynomially many elements, and the Borel-Cantelli lemma, we may show that with probability 1,

$$\sup_{t \in \mathcal{T}} \max_{a + Ch \le x \le b - Ch} \left| \hat{g}_t(x) - g_t(x) \right| = O(\eta). \tag{5.5}$$

Now consider a generalized form of the estimator $\hat{g}_t(x)$ in which, rather than generating pseudo-data by reflecting the real data through points $(a, \tilde{g}_t(a))$ and $(b, \tilde{g}_t(b))$, we reflect through $(a, \xi_t(a))$ and $(b, \xi_t(b))$, where $\xi_t(x)$ is nondecreasing in t for x = a, b. Let $\hat{g}_{\xi_t,t}$ denote the resulting version of \hat{g}_t . Using the linearity of Nadaraya-Watson estimators we may, for $|x - a| \leq Ch$, write $\hat{g}_{\xi_t,t}(x) = \hat{g}_{g_t,t}(x) + \{\xi_t(a) - g_t(a)\} \zeta_t(x)$, where the function ζ_t does not depend on choice of ξ_t . Arguments leading to (5.5) may be employed to prove that with probability 1,

$$\sup_{t \in \mathcal{T}} \sup_{|x-a| \le Ch} |\hat{g}_{g_t,t}(x) - g_t(x)| = O(\eta), \quad \sup_{t \in \mathcal{T}} \sup_{|x-a| \le Ch} |\zeta_t(x)| = O(1).$$

Making the choice of ξ_t at (5.3), and noting that (5.4) holds for this selection, we deduce that

$$\sup_{t \in \mathcal{T}} \max_{|x-a| \le Ch} \left| \hat{g}_t(x) - g_t(x) \right| = O(\eta). \tag{5.6}$$

A similar property holds at the other boundary. Combining that result with (5.5) and (5.6), we deduce Theorem 3.3.

Derivation of Theorem 3.4 may similarly be based on application of the Borel-Cantelli lemma, this time using Markov's inequality and moment bounds, as well as techniques from the proof of Theorem 3.3, to prove that for some $C_1 > 0$ and all $C_2 > 0$,

$$P\left[\int \int \left\{ \widehat{F}(t|x) - F(t|x) \right\}^2 dt \, dx > C_1 \left\{ (nh)^{-1} + h^4 \right\} \right] = O(n^{-C_2}).$$

6. Concluding remarks

The proposed order-preserving nonparametric regression algorithm provides a first solution to a problem that was previously not tractable, namely to ensure that nonparametric regression function estimators respect order relationships within the responses, in the interior of the range of the covariate as well as near or at endpoints of the range. We illustrate the importance of the problem and the efficacy of the proposed solution in the case of conditional distribution function estimation. Order-preserving estimation is here a prerequisite for defining bona fide conditional distribution function estimates.

The problem of crossing quantile estimators has been noted and addressed before in linear regression models (He, 1997). A comprehensive solution as that given here has not previously been provided. Further relevant applications include the construction of prediction intervals for new observations that are made near endpoints as well as the change-point problem.

We have shown that no linear method, and this includes practically all commonly used nonparametric regression methods, has the property of being order-preserving on the whole domain of the predictor variable. The proposed nonlinear procedure works well and has been shown to possess attractive asymptotic properties. Topics of interest for future research are the development of other order-preserving nonparametric regression methods and an investigation of asymptotic distributions.

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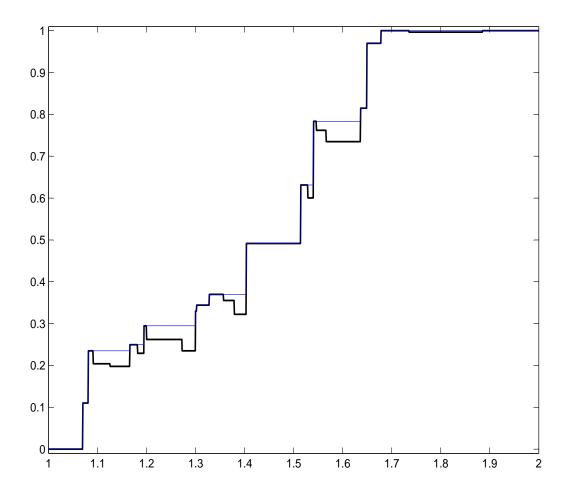


Figure 1: Filling in the "valleys" of the initial distribution function estimate $\widehat{F}_{LL}(\cdot|b)$ obtained by local linear fitting at a right endpoint b (solid line) results in a monotone increasing estimate $\widetilde{F}(t|b)$ (thin line), as t increases (Simulated example with n=100 data.)

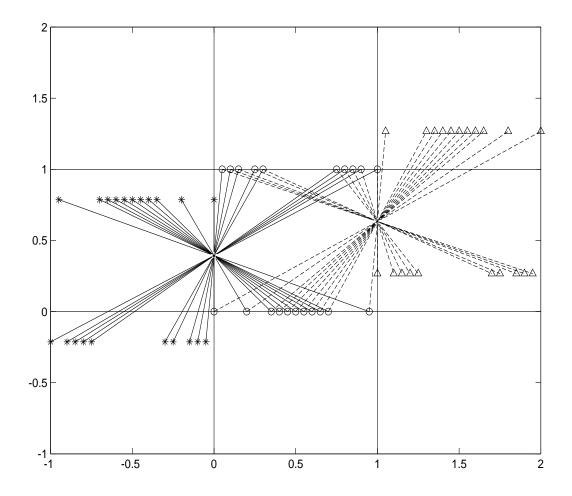


Figure 2: Generation of pseudo-data \mathcal{X}'_t by reflecting original data \mathcal{X}_t (confined to domain [a,b]=[0,1]) at the points $(0,\tilde{F}(t|0))$ and $(1,\tilde{F}(t|1))$. The data (X_i,Y_{ti}) illustrated here were simulated, using sample size n=20 and a single value for t. The response variables are indicators $Y_{ti}=I(Z_i\leq t)$, as used for the application to estimating a conditional distribution function.

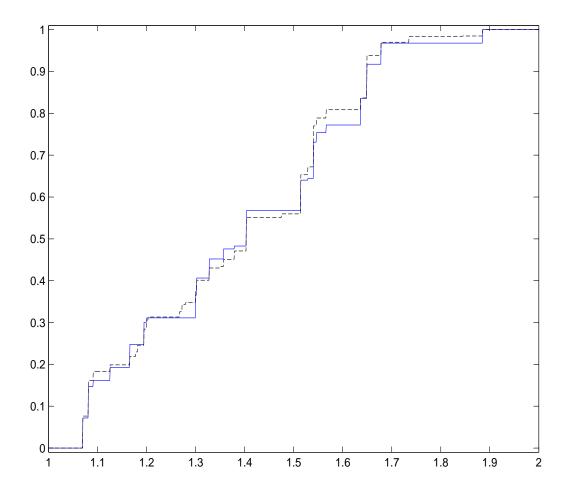


Figure 3: Comparison of monotonized intermediate conditional distribution function estimate $\tilde{F}(\cdot,x)$ (solid) and the final estimate $\hat{F}(\cdot,x)$ (dashed), constructed from the pseudo-data \mathcal{X}_t' obtained in the reflection step. Here for simulated data with n=100, h=0.2 when estimating at the point x=.95 near the right endpoint at b=1.

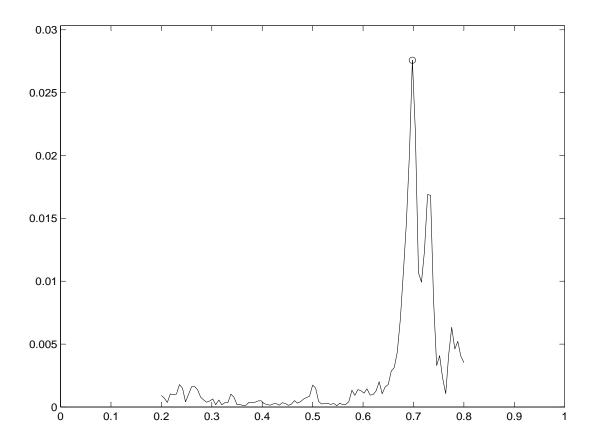


Figure 4: The change-point detection function $\Delta(\cdot)$ for simulated variance change data (n = 1000, h = 0.2, fixed design case). The peak selected for the change-point estimate is highlighted.

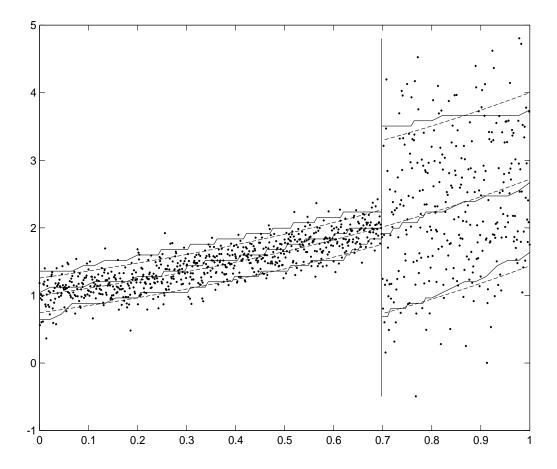


Figure 5: The estimated conditional quantile functions for the variance change data (h = 0.2, n = 1000). Indicated are the 0.1, 0.5 and 0.9 estimated (solid) and true (dashed) quantile curves. Estimated curves are adapted to the estimated change-point location.

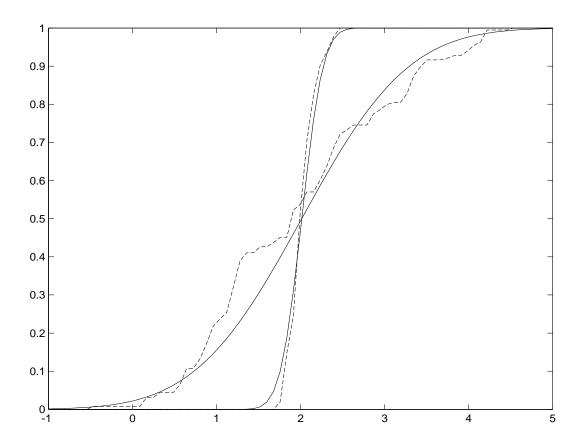


Figure 6: The estimated conditional distribution functions $\hat{F}_{-}(t|\hat{\theta})$ (steep dashed function) and $\hat{F}_{+}(t|\hat{\theta})$ (less steep dashed function), and the true Gaussian conditional distribution functions $F_{-}(t|\theta)$ (steep solid function) and $F_{+}(t|\theta)$ (less steep solid function). The distribution function estimates use only data on left or right side of the estimated change-point.

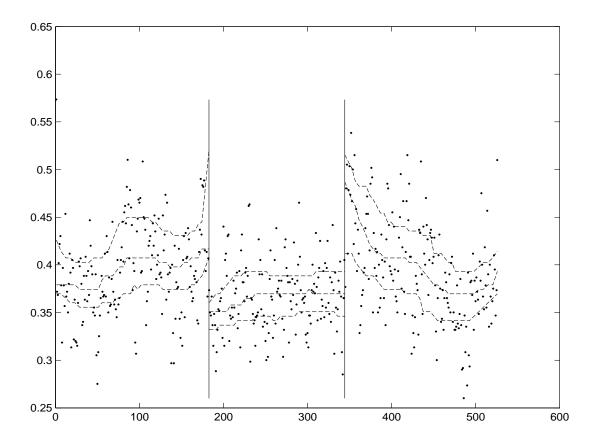


Figure 7: The estimated order-preserving conditional quantile functions (h = 50kbp) for the S. cerevisiae III DNA sequence, indicated by estimated 0.25, 0.5 and 0.75 quantile curves, and adapted to the two estimated change-point locations.