

AD-A191 990

SYMMETRIZED NEAREST NEIGHBOR REGRESSION ESTIMATES(U)
NORTH CAROLINA UNIV AT CHAPEL HILL DEPT OF STATISTICS
R J CARROLL ET AL. DEC 87 NMS-1742 AFOSR-TR-88-0201

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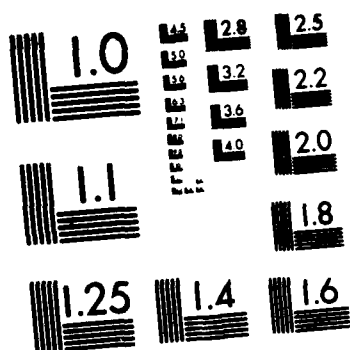
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AD-A191 998

ORT DOCUMENTATION PAGE

UNCLASSIFIED

DTIC
SELECTED
MAR 04 1988

2b. SECURITY CLASSIFICATION AND DECLASSIFICATION/DOWNGRADING SCHEDULE

1b. RESTRICTIVE MARKINGS
3. DISTRIBUTION/AVAILABILITY OF REPORT
Approved for public release;
distribution unlimited.

4. PERFORMING ORGANIZATION REPORT NUMBER(S)
MIMEO SERIES #1742

5. MONITORING ORGANIZATION REPORT NUMBER(S)
AFOSR-TR- 88-0201

6a. NAME OF PERFORMING ORGANIZATION
Univ. of NC - Chapel Hill

6b. OFFICE SYMBOL
(If applicable)

7a. NAME OF MONITORING ORGANIZATION
Air Force Office of Scientific Research

6c. ADDRESS (City, State and ZIP Code)
Statistics Department, UNC-CH
Chapel Hill, NC 27514

7b. ADDRESS (City, State and ZIP Code)
Same as 8c

8a. NAME OF FUNDING/SPONSORING ORGANIZATION
AFOSR

8b. OFFICE SYMBOL
(If applicable)
DM

9. PROCUREMENT INSTRUMENT IDENTIFICATION NUMBER
AFOSR-F49620-85-C-0144

9a. ADDRESS (City, State and ZIP Code)
Bolling Air Force Base
Washington, DC 20332

10. SOURCE OF FUNDING NOS.

11. TITLE (Include Security Classification)
"SYMMETRIZED NEAREST NEIGHBOR REGRESSION ESTIMATES"

PROGRAM ELEMENT NO. PROJECT NO. TASK NO. WORK UNIT NO.
61102F 2304 AS

12. PERSONAL AUTHOR(S)
CARROLL, R.J. and HARDLE, W.

13a. TYPE OF REPORT
Technical journal

13b. TIME COVERED
FROM 9/87 TO 9/88

14. DATE OF REPORT (Yr., Mo., Day)
December 1987

15. PAGE COUNT
8 pages

16. SUPPLEMENTARY NOTATION

17. COSATI CODES
FIELD GROUP SUB. GR.

18. SUBJECT TERMS (Continue on reverse if necessary and identify by block number)
Nonparametric regression, kernel regression, nearest neighbor regression, bias, mean squared error

19. ABSTRACT (Continue on reverse if necessary and identify by block number)
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20. DISTRIBUTION/AVAILABILITY OF ABSTRACT
UNCLASSIFIED/UNLIMITED SAME AS RPT. OTIC USERS

21. ABSTRACT SECURITY CLASSIFICATION

22a. NAME OF RESPONSIBLE INDIVIDUAL
Major Brian Woodruff

22b. TELEPHONE NUMBER
(Include Area Code)
(202) 767-5026

22c. OFFICE SYMBOL
DM

SYMMETRIZED NEAREST NEIGHBOR REGRESSION ESTIMATES

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AFOSR-TR- 88 - 0201



Accession For	
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DTIC TAB	<input type="checkbox"/>
Unannounced	<input type="checkbox"/>
Justification	
By	
Distribution /	
Availability Codes	
Dist	Avail and/or Special
A-1	

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ABSTRACT

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We consider univariate nonparametric regression. Two standard nonparametric regression function estimates are kernel estimates and nearest neighbor estimates. Mack⁹(1981) noted that both methods can be defined with respect to a kernel or weighting function, and that for a given kernel and a suitable choice of bandwidth, the optimal mean squared error is the same asymptotically for kernel and nearest neighbor estimates. Yang¹(1981) defined a new type of nearest neighbor regression estimate using the empirical distribution function of the predictors to define the window over which to average. This has the effect of forcing the number of neighbors to be the same both above and below the value of the predictor of interest; we call these symmetrized nearest neighbor estimates. The estimate is a kernel regression estimate with ^g"predictors"² given by the empirical distribution function \hat{F} of the true predictors. We show that for estimating the regression function at a point, the optimum mean squared error of this estimate differs from that of the optimum mean squared error for kernel and ordinary nearest neighbor estimates. No estimate dominates the others. They are asymptotically equivalent with respect to mean squared error if one is estimating the regression function at a mode of the predictor.

Key Words and Phrases: Nonparametric regression, kernel regression, nearest neighbor regression, bias, mean squared error.

Section 1: Introduction

We consider nonparametric regression with a random univariate predictor. Let (X, Y) be a bivariate random variable with joint distribution H , and denote the regression function of Y on X by $m(x) = E(Y | X = x)$. If it exists, let f_x denote the marginal density of X . A sample of size n is taken, (y_i, x_i) for $i = 1, \dots, n$. Two common estimates of the regression function are the Nadaraya-Watson kernel estimate and the nearest neighbor estimate, see Nadaraya (1964), Watson (1964) and Stute (1984) for the former, and Mack (1981) for the latter. Fix x_0 and suppose we wish to estimate $m(x_0)$. The kernel and nearest neighbor estimates are defined as follows. Let K be a nonnegative even density function.

Kernel Estimates Let h_{ker} be a bandwidth depending on n . Then the kernel estimate is

$$(1) \quad \hat{m}_{ker}(x_0) = \frac{\sum_{i=1}^n y_i K\left(\frac{x_i - x_0}{h_{ker}}\right)}{\sum_{i=1}^n K\left(\frac{x_i - x_0}{h_{ker}}\right)}$$

Nearest Neighbor Estimates Let $k = k(n)$ be a sequence of positive integers, and let R_n be the Euclidean distance between x_0 and its k th nearest neighbor. Then the nearest neighbor estimate is

$$(2) \quad \hat{m}_{kNN}(x_0) = \frac{\sum_{i=1}^n y_i K\left(\frac{x_i - x_0}{R_n}\right)}{\sum_{i=1}^n K\left(\frac{x_i - x_0}{R_n}\right)}$$

Under differentiability conditions on the marginal density f_x , Mack has shown that the asymptotically optimal versions of the kernel and nearest neighbor estimates have the same behavior. Let $m^{(j)}$ and $f_x^{(j)}$ denote the j th derivative of m and f_x respectively. If $c_K = \int K^2(x)dx$ and $d_K = \int x^2 K(x)dx$, remembering that K is symmetric, the kernel estimate has bias

$$(3) \quad bias_{ker} = h_{ker}^2 d_K \frac{m^{(2)}(x_0)f_x(x_0) + 2m^{(1)}(x_0)f_x^{(1)}(x_0)}{2f_x(x_0)} + o(h_{ker}^2)$$

and variance

$$(4) \quad var_{ker} = c_K Var(Y | X = x_0) / (nh_{ker} f_x(x_0)) + o((nh_{ker})^{-1}).$$

There is obviously a bias versus variance tradeoff here, so that if one wants to achieve the minimum mean squared error, the optimal bandwidth is $h_{ker} \sim n^{-1/5}$ and the optimal mean squared error is of order $O(n^{-4/5})$. The formulae for bias and variance of the k th nearest neighbor estimate are the same as in (3) and (4) if one substitutes $2f_x(x_0)nh_{ker}$ for k .

Let F denote the distribution function of X , and let F_n denote the empirical distribution of the sample from X . Let $h_{,nn}$ be a bandwidth tending to zero. The estimate proposed by Yang (1981) and studied by Stute (1984) is

$$(5) \quad \hat{m}_{,nn}(x_0) = (nh_{,nn})^{-1} \sum_{i=1}^n y_i K\left(\frac{F_n(x_i) - F_n(x_0)}{h_{,nn}}\right).$$

The nearest neighbor estimate defines neighbors in terms of the Euclidean norm, which in this case is just absolute difference. The estimate (5) is also a nearest neighbor estimate, but now neighbors are defined in terms of distance based on empirical distribution function. This makes for computational efficiency if the uniform kernel is used. A direct application of (5) would result in $O(n^2h)$ operations, but using updating as the window moves over the span of the x 's results in $O(n)$ operations. Other smooth kernels can be computed efficiently by iterated smoothing, i.e., higher order convolution of the uniform kernel. Another possible device is the Fast Fourier transform (Härdle, 1987). Since the difference between (2) and (5) is that (5) picks its neighbors symmetrically, we call it a symmetrized nearest neighbor estimate. Note that \hat{m}_{kNN} always averages over a symmetric neighborhood in the x -space, but may have an asymmetric distribution of x points in this neighborhood. By contrast, $\hat{m}_{,nn}$ always averages over the same amount of points left and right of x_0 , but may in effect average over an asymmetric neighborhood in the x -space. The estimate $\hat{m}_{,nn}$ has an intriguing relationship with the k -NN estimator used by Friedman (1986). The variable span smoother proposed by Friedman uses the same type of neighborhood as does $\hat{m}_{,nn}$ and is used as an elementary building block for ACE, see Breiman and Friedman (1985). The estimate (5) also looks appealingly like a kernel regression estimate of Y against not X but rather $F_n(X)$. Define

$$(6) \quad \bar{m}_{,nn}(x_0) = h_{,nn}^{-1} \int m(x) K\left(\frac{F(x) - F(x_0)}{h_{,nn}}\right) dx.$$

Then Stute shows that as $n \rightarrow \infty$, $h_{,nn} \rightarrow 0$ and $nh_{,nn}^3 \rightarrow \infty$,

$$(7) \quad (nh_{,nn})^{1/2} (\hat{m}_{,nn}(x_0) - \bar{m}_{,nn}(x_0)) \Rightarrow Normal(0, c_K Var(Y | X = x_0)).$$

This has the form (4) as long as $h_{,nn} = h_{ker} f_x(x_0)$. With this choice of $h_{,nn}$, Stute's estimate has the same limit properties as a kernel or ordinary nearest

neighbor estimate as long as its bias term satisfies (3). Stute shows that the bias is of order $O(h_{n,n}^2)$, although he does not give an asymptotic formulae. It is in fact easy to show that the bias satisfies to order $o(h_{n,n}^2)$

$$(8) \quad bias_{n,n} = h_{n,n}^2 d_K \frac{m^{(2)}(x_0)f_x(x_0) - m^{(1)}(x_0)f_x^{(1)}(x_0)}{2f_x^2(x_0)}.$$

Comparison of (3) and (8) shows that even when the variances of all three estimates are the same (the case $h_{n,n} = h_{ker} f_x(x_0)$), the bias properties differ unless

$$m^{(1)}(x_0)f_x^{(1)}(x_0) = 0.$$

Otherwise, the optimal choice of bandwidth for the kernel and ordinary nearest neighbor estimates will lead to a different mean squared error than what obtains for the symmetrized nearest neighbor estimate.

The preceding discussion presumed that we are interested in estimating the regression function only at the point x_0 and that bandwidth was chosen locally so as to minimize asymptotic mean squared error. In practice, one is usually interested in the regression curve over an interval, and the bandwidth is chosen globally, see for example Härdle, Hall and Marron (1988). Inspection of (3), (4) and (8) shows the usual tradeoff between kernel and nearest neighbor estimates: in the tails of the distribution of x , the former are more variable but less biased.

The symmetrized nearest neighbor estimate is a kernel estimate based on transforming the x data by F_n . Other transformations are possible, e.g., $\log(x)$. In general, if we transform by $w = G(x)$, if $m_w(w) = m(x)$ and w has density f_w , then the bias and variance properties of the resulting kernel estimate are given by (3)-(4) in m_w and f_w , the translation to f_x and m being immediate by the chain rule.

An Example

For illustrative purposes we use a large data set ($n=7125$) of the relationship of $Y =$ expenditure for potatoes versus $X =$ net income of British households (in tenth of a pence) in 1973. The data come from the *Family Expenditure Survey, Annual Base Tapes 1968-1988*, Department of Employment, Statistics Division, Her Majesty's Stationary Office, London, and were made available by the ESRC Data Archive at the University of Essex. See Härdle (1988, Chapter 1) for a discussion. For these data, we used the quartic kernel

$$K(u) = \frac{15}{16}(1 - u^2)^2 I(|u| \leq 1).$$

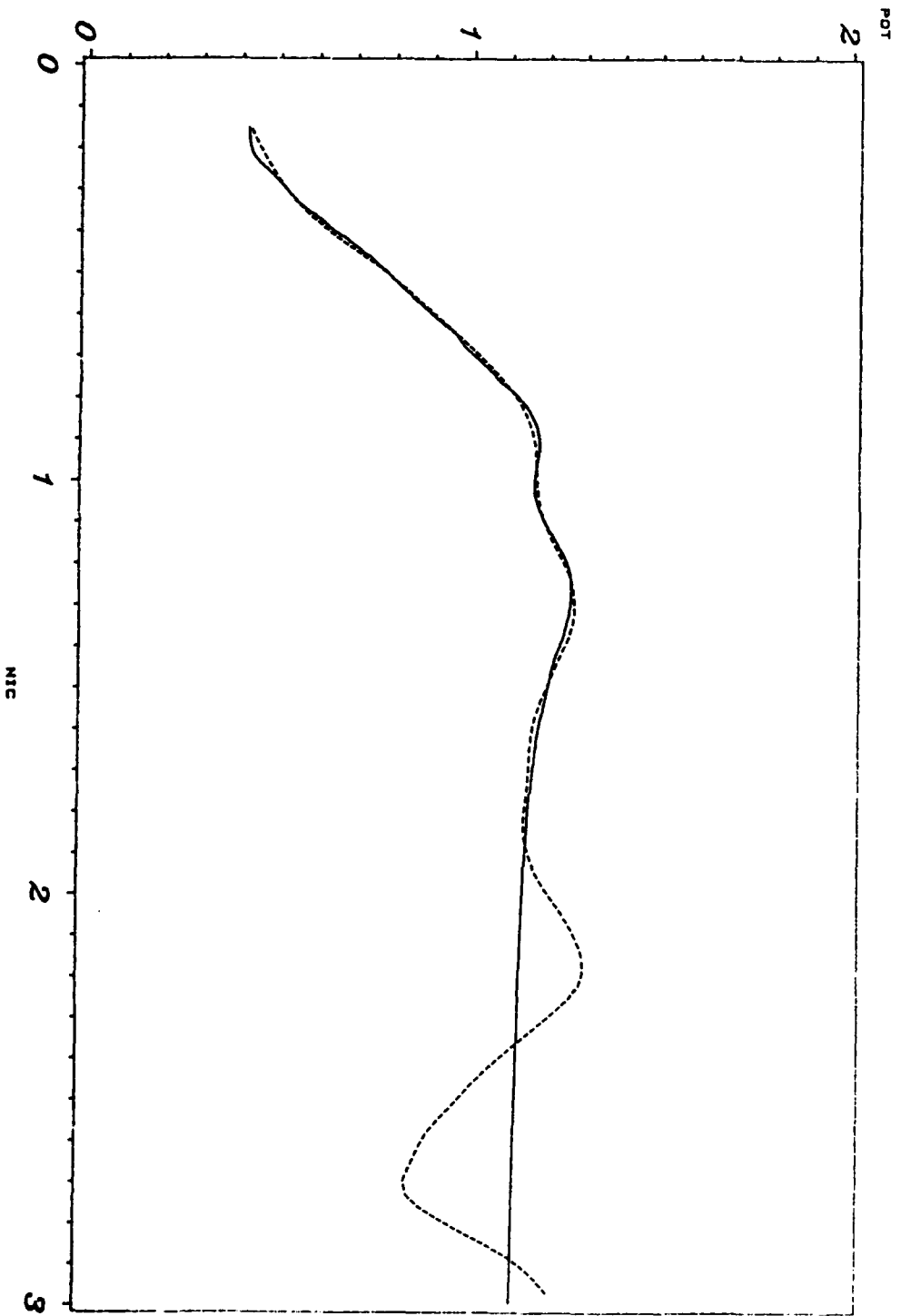
We computed the ordinary kernel estimate (1) and the symmetrized nearest neighbor estimate (5), the bandwidths being selected by crossvalidation, see Härdle and Marron (1985). The crossvalidated bandwidths were $h_{ker} = 0.25$ on the scale (0,3) of Figure 1 and $h_{nn} = 0.15$ on the F_n scale. The resulting regression curves are plotted in Figure 1. The two curves are similar for $x \leq 1$, which is where most of the data lie. There is a sharp discrepancy for larger values of x , the kernel estimate showing evidence of a bimodal relationship and the symmetrized nearest neighbor estimate indicating either an asymptote or even a slight decrease as income rises. In the context, the latter seems to make more sense economically and looks quite similar to the curve in Hildenbrand and Hildenbrand (1986). Statistically, it is in this range of the data that the density f_x takes on small values, which is exactly when we expect the biggest differences in the estimates, i.e., the kernel estimate should be more variable but less biased.

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