

Near-Linear Time Local Polynomial Nonparametric Estimation with Box Kernels

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Local polynomial regression (Fan and Gijbels 1996) is an important class of methods for nonparametric density estimation and regression problems. However, straightforward implementation of local polynomial regression has quadratic time complexity which hinders its applicability in large-scale data analysis. In this paper, we significantly accelerate the computation of local polynomial estimates by novel applications of multi-dimensional binary indexed trees (Fenwick 1994). Both time and space complexity of our proposed algorithm is nearly linear in the number of input data points. Simulation results confirm the efficiency and effectiveness of our proposed approach.

Key words: local polynomial regression, nonparametric density estimation, binary indexed trees, hashing

1. Introduction

Big data analytics has become essential for modern operations research and operations management applications (Choi et al. 2018, Hazen et al. 2018, Mišić and Perakis 2019). Statistics methods, such as nonparametric density and function estimation (Larry 2006, Tsybakov 2009, Friedman et al. 2001), play important roles in the prediction of economic trends like loan management and market profit prediction (Györfi et al. 2006), as well as exploratory data analysis as preliminary steps to operations management problems, such as the understanding and estimation of customers' demand or preferences in revenue management applications. Naturally, big data scenarios pose unique challenges from *computing* aspects, as many classical statistical computational routines (especially nonparametric statistical methods) are computationally heavy and not scalable to large amounts of data.

The focus of this paper is on nonparametric density estimation and regression problems. Let $\mathcal{X} \subseteq \mathbb{R}^d$ be a compact domain in \mathbb{R}^d , which is conventionally taken to be the unit cube

$[0, 1]^d$ for convenience. In the *nonparametric density estimation* problem, n independent samples $X_1, \dots, X_n \in \mathcal{X}$ are obtained as

$$X_1, \dots, X_n \stackrel{i.i.d.}{\sim} f_0, \tag{1}$$

where f_0 is the density of an unknown distribution P_0 supported on \mathcal{X} . In the *nonparametric regression* problem, on each of n “design points” $X_1, \dots, X_n \in \mathcal{X}$ a “response” or “measurement” Y_i is obtained according to the model

$$Y_i = m_0(X_i) + \xi_i, \quad i = 1, \dots, n, \tag{2}$$

where $m_0 : \mathcal{X} \rightarrow \mathbb{R}$ is an unknown regression model of interest, and $\{\xi_i\}$ are independent sub-Gaussian noise variables satisfying $\mathbb{E}[\xi_i | X_i] = 0$. The objective in both nonparametric estimation problems is to construct estimates \hat{f}_n or \hat{m}_n such that the *mean-square error (MSE)*

$$\int_{\mathcal{X}} |\hat{f}_n(x) - f_0(x)|^2 dx \text{ or } \int_{\mathcal{X}} |\hat{m}_n(x) - m_0(x)|^2 dx$$

is minimized.

The nonparametric density estimation and regression problems have a long history of study, dating back to the 1920s (Whittaker 1922). A large family of methods have been developed and their properties analyzed, including kernel smoothing (Friedman et al. 2001, Györfi et al. 2006), spline smoothing (Reinsch 1967, Geer 2000, Green and Silverman 1993), wavelet smoothing (Donoho et al. 1998, Donoho and Johnstone 1994, Härdle et al. 2012) and local polynomial regression (Fan and Gijbels 1992, Fan 1993, Fan and Gijbels 1996).

In this paper, we concentrate on the local polynomial regression method introduced in (Fan and Gijbels 1992, Fan 1993, Fan and Gijbels 1996). Compared to its competitors, local polynomial regression has the benefits of being adaptive to non-uniform design densities and regression functions of unbounded values (Hastie and Loader 1993). In Sec. 2 we give a succinct description of these methods and also summarize some of their basic properties.

While the statistical properties of local polynomial regression are well understood, computational efficiency has been less studied. In particular, straightforward implementation of local polynomial regression typically has *quadratic* time complexity $O(sn)$ to calculate $\hat{f}_n(z_i)$ or $\hat{m}_n(z_i)$ on s “testing points” $z_1, \dots, z_s \in \mathcal{X}$, which is prohibitively slow for analysis of large data sets. We give an illustrative example in Figure 1, which shows that the

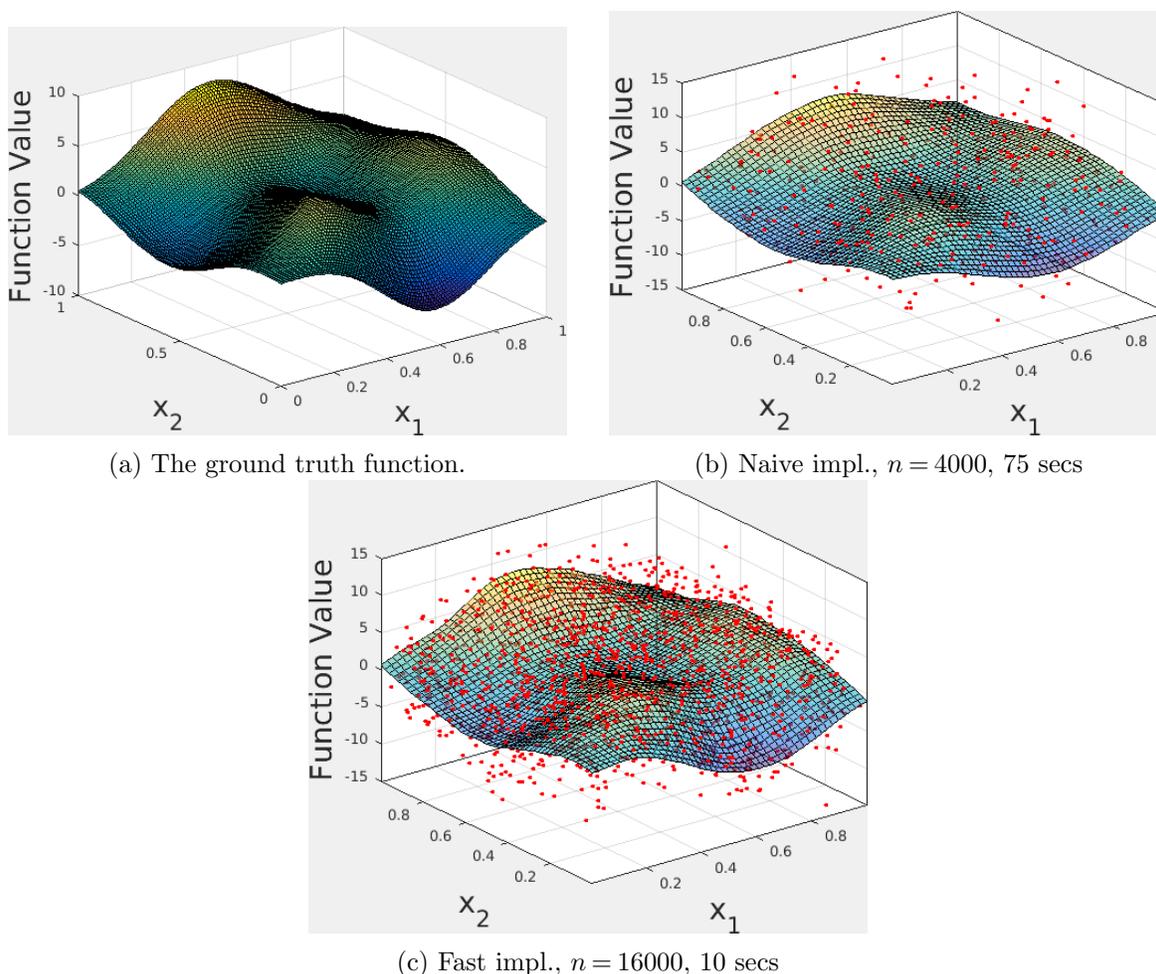


Figure 1 Illustration of local polynomial regression with naive and fast implementation for fitting a two dimensional smooth function $f(x, y) = 3(1 - x)^2 e^{-x^2 - (y+1)^2} - 10(0.2x - x^3 - y^5) e^{-x^2 - y^2} - e^{-(x+1)^2 - y^2} / 3$. Red points are observations (training points), down sampled $10\times$ for better visualization. The number of testing points is large ($\sim 1,000,000$), as reconstruction of the entire function is desired. Under such settings, the naive implementation (middle panel) takes 75 secs to process $n = 4000$ observations (training points), while our fast implementation (Algorithm 1, right panel) only takes 10 secs to process $n = 16000$ observations. As a result, there is a visible difference between the fitted curves under the naive and the fast implementation, because the naive implementation can only process a small number of observations under given time budget and therefore needs to significantly “over-smooth” the data, leading to inaccurate function reconstruction. Indeed, the mean-square errors of the naive and fast implementation are 9×10^{-3} and 2×10^{-3} respectively, which is a near $5\times$ gap.

computational bottleneck of the naive implementation of local polynomial regression significantly restricts the number of observations (training points) it processes under given time budget, leading to inaccurate function estimates.

The apparent difficulties of computationally efficient local polynomial regression motivate the following question:

QUESTION 1. Given n training data points $\{(X_i, Y_i)\}_{i=1}^n$ and s testing points $z_1, \dots, z_s \in \mathcal{X}$, can we compute local polynomial estimates $\hat{f}_n(z_1), \dots, \hat{f}_n(z_s)$ or $\hat{m}_n(z_1), \dots, \hat{m}_n(z_s)$ in $O((n+s)\text{poly log } n)$ time?

Essentially, Question 1 concerns estimation algorithms whose time complexity is *nearly linear* in the total number of training and testing points $n+s$, apart from possible polylogarithmic factors. On the other hand, a linear dependency on $n+s$ is clearly necessary as the number of inputs is already on the order of $n+s$.

We give an affirmative answer to Question 1 in this paper by accelerating local polynomial regression using efficient data structures. In particular, applying a multi-dimensional extension of binary indexed trees (Fenwick 1994) we are able to reduce the computation time on each testing point from $O(n)$ to $O(\log^d n)$. Furthermore, to avoid space complexity growing exponentially with dimension d , we consider a *lazy allocation* strategy that allocates memory on the fly with the help of a Hash table, which achieves near-linear space complexity. Our computations of all local polynomial estimates are exact, and therefore all statistical properties of local polynomial regression are automatically preserved.

Finally, we remark that certain existing nonparametric estimation methods can also achieve near-linear time complexity, such as the B-spline (De Boor 1978) and/or falling factorial basis (Wang et al. 2014) construction in smoothing splines and block thresholding of wavelet coefficients (Cai 1999). However, both smoothing spline and wavelet thresholding (shrinkage) methods become very complicated for multi-dimensional and non-uniformly spaced data points. For example, the extension of smoothing splines to higher dimension requires complicated constructions of the “thin-plate” splines, and in the case of wavelet smoothing the basis functions are complicated and difficult to compute when design points are not evenly spaced. On the other hand, the local polynomial regression method easily handles both cases of multi-dimensionality and unevenly spaced design points without much additional complexity.

2. Local polynomial regression

In this section we give a succinct description of local polynomial regression (Fan and Gijbels 1996) in the context of nonparametric estimation problems, with high-level summarization of its properties.

Let $k \in \mathbb{N}$ be the desired polynomial degree used in estimation. Practical choices of k are small non-negative integers, such as $k=0$ (local mean averaging), $k=1$ (local linear

regression) and $k = 2$ (local quadratic regression). For any $z \in \mathbb{R}^d$, define the polynomial mapping $\psi_z : \mathbb{R}^d \rightarrow \mathbb{R}^D$, $D = 1 + d + \dots + d^k$ as

$$\begin{aligned} \psi_z(x) := & [1, x_1 - z_1, \dots, x_d - z_d, (x_1 - z_1)^2, (x_1 - z_1)(x_2 - z_2), \dots, (x_d - z_d)^2, \\ & \dots, (x_1 - z_1)^k, \dots, (x_d - z_d)^k]. \end{aligned}$$

At a higher level, the polynomial mapping $\psi_x(\cdot)$ is an expansion of basis of degree- k polynomials on \mathbb{R}^d , appropriately offset so that $\psi_z(z) = [1, 0, \dots, 0]$. As we shall see immediately, the mapping ψ_z plays a fundamental role in local polynomial regression methods.

We first consider the regression problem $Y_i = m_0(X_i) + \xi_i$. We start by introducing the concepts of *kernel functions* and *bandwidths*, which are crucial to almost every nonparametric estimation method:

1. A *kernel function* $K : \mathbb{R} \rightarrow \mathbb{R}$ that satisfies constraints $\int_{-\infty}^{\infty} K(u)du = 1$, $\int_{-\infty}^{\infty} K(u)udu = 0$ and $\int_{-\infty}^{\infty} K^2(u)du < \infty$ is used to “average” neighboring data points in a certain manner. Common kernel functions include the box kernel $K(u) = \mathbb{I}[|u| \leq 1/2]$, the Gaussian kernel $K(u) = \frac{1}{\sqrt{2\pi}}e^{-u^2/2}$ and the Epanechnikov kernel $K(u) = \frac{3}{4\sqrt{5}} \max(0, 1 - u^2/5)$.
2. A *bandwidth* parameter $h > 0$ is used to control the size of the “neighborhood” of a certain test point $z \in \mathcal{X}$ in which training points are incorporated and smoothed. A small bandwidth h will have fewer effective training points rendering the variance of the resulting estimate large, while a large bandwidth h tends to “over-smooth” the unknown function over a large domain and therefore leading to larger estimation bias.

To estimate the value of the unknown regression function m_0 at a specific testing point z , first solve a weighted least-squares problem ¹

$$\hat{\theta}_n = \arg \min_{\theta \in \mathbb{R}^D} \sum_{i=1}^n (Y_i - \theta^\top \psi_z(X_i))^2 K\left(\frac{\|z - X_i\|_\infty}{h}\right) \quad (3)$$

where $\|z - X_i\|_\infty = \max_{1 \leq j \leq d} |z_j - X_{ij}|$. Afterwards, $\hat{m}_n(z)$ is taken to be $\hat{\theta}_n^\top \psi_z(z)$, which corresponds to the first component of $\hat{\theta}_n$.

¹ Although in the literature the ℓ_2 norm $\|z - X_i\|_2 = \sqrt{\sum_{j=1}^d (z_j - X_{ij})^2}$ is more commonly used, replacing the ℓ_2 norm with ℓ_∞ does not affect the statistical properties of $\hat{\theta}_n$, because ℓ_2 and ℓ_∞ are equivalent norms when dimension d is fixed.

EXAMPLE 1. When $K(\cdot)$ is taken to be the box kernel $K(u) = \mathbb{I}[|u| \leq 1/2]$, Eq. (3) can be re-formulated as

$$\hat{g}_n = \arg \min_{g \in \mathcal{P}_k} \sum_{X_i \in B_h(z)} (Y_i - g(X_i))^2$$

where \mathcal{P}_k is the class of all degree- k polynomials on \mathbb{R}^d and $B_h(z) = \{u \in \mathcal{X} : \|u - z\|_\infty \leq h/2\}$ denotes the neighborhood of z with radius h . The re-formulation of \hat{g}_n is a clear interpretation of the polynomial fitting (in \mathcal{P}_k) and the local properties (in $B_h(z)$).

The density estimation problem is slightly more involved than local polynomial regression. Here we adopt the approach in (Cattaneo et al. 2017) by re-casting the density estimation problem as a regression problem. For every $X_i \in \mathcal{X}$ define empirical cumulative density function (CDF)

$$\hat{F}(X_i) := \frac{1}{n} \sum_{j=1}^n \mathbb{I}[X_{j1} \leq X_{i1}, \dots, X_{jd} \leq X_{id}] \quad (4)$$

that approximates the true CDF $F(X_i) = \int_{\mathcal{X}} \mathbb{I}[u_1 \leq X_{i1}, \dots, u_d \leq X_{id}] f_0(u) du$. Afterwards, a local polynomial fit of \hat{F} is computed as

$$\hat{\beta}_n = \arg \min_{\beta \in \mathbb{R}^D} \sum_{i=1}^n (\hat{F}(X_i) - \theta^\top \psi_z(X_i))^2 K\left(\frac{\|z - X_i\|_\infty}{h}\right).$$

Because $f_0 = \partial^d F / \partial x_1 \cdots \partial x_d$, an estimate $\hat{f}_n(z)$ can be obtained by reading off the component in $\hat{\beta}_n$ corresponding to $(z_1 - x_1)(z_2 - x_2) \cdots (z_d - x_d)$ multiplied by $d!$. Note that $k \geq d$ is required for this density estimation method.

Local polynomial regression enjoys a wide range of desired properties. When bandwidths h are properly tuned (for example by cross-validation), local polynomial regression is minimax optimal when the underlying model f_0 or m_0 belongs to Hölder or Sobolev smoothness classes. In addition, when bandwidths are selected *locally*, the resulting estimation is optimal even for spatially heterogeneous functions (Lepski et al. 1997). The local polynomial regression estimator also adapts to non-uniform and non-smooth design densities and boundaries (Fan and Gijbels 1992, 1996, Cheng et al. 1997, Hastie and Loader 1993), properties that do not hold for kernel smoothing estimators.

3. Our method

We describe our proposed method for local polynomial regression with the box kernel that achieves $O((n+s) \log^d n)$ time complexity and $O(n \log^d n)$ space complexity, which is the main contribution of this paper.

We start by formulating sufficient statistics required to compute local polynomial estimates, and giving a simple nearly linear-time algorithm for the univariate case $d = 1$ as a warm-up exercise. We then proceed with a formal discretization argument for higher dimensions, and explain how binary indexed trees can be applied to enable fast calculations. Finally, a lazy memory allocation scheme is employed to avoid memory explosion in high-dimensional binary indexed trees.

3.1. Sufficient statistics of local polynomial regression

When the box kernel $K(u) = \mathbb{I}[|u| \leq 1/2]$ is used, the local polynomial regression formulation in Eq. (3) is an ordinary least squares (OLS) problem on $\mathcal{B}(z, h) := \{(X_i, Y_i) : \|X_i - z\|_\infty \leq h/2\}$, where $z \in \mathcal{X}$ is the testing point. The solution $\widehat{\theta}_n$ admits the following closed form:

$$\widehat{\theta}_n = \left[\sum_{\mathcal{B}(z, h)} \psi_z(X_i) \psi_z(X_i)^\top \right]^{-1} \left[\sum_{\mathcal{B}(z, h)} Y_i \psi_z(X_i) \right]. \quad (5)$$

Recall that $\psi_z(X_i)$ is a multivariate polynomial function in X_i . The sufficient statistics required to compute Eq. (5) can then be organized as follows:

1. $\sum_{(X_i, Y_i) \in \mathcal{B}(z, h)} X_{i1}^{j_1} X_{i2}^{j_2} \cdots X_{id}^{j_d}$ for $j_1 + \cdots + j_d \leq 2k$;
2. $\sum_{(X_i, Y_i) \in \mathcal{B}(z, h)} Y_i X_{i1}^{j_1} \cdots X_{id}^{j_d}$ for $j_1 + \cdots + j_d \leq k$.

Let M be the total number of terms summarized above. For each $\ell \in \{1, 2, \dots, M\}$, define $T_\ell(X_i, Y_i)$ to be either $X_{i1}^{j_1} X_{i2}^{j_2} \cdots X_{id}^{j_d}$ or $Y_i X_{i1}^{j_1} \cdots X_{id}^{j_d}$, where $j_1 + \cdots + j_d \leq 2k$ or $j_1 + \cdots + j_d \leq k$ are indices corresponding to term $\ell \leq M$. The terms $T_\ell(X_i, Y_i)$ for $\ell \leq M$ are then *sufficient statistics* required to compute the local polynomial estimate $\widehat{\theta}_n$ in Eq. (5).

Once the sufficient statistics $\mathcal{T}_\ell(X_i, Y_i)$, $(X_i, Y_i) \in \mathcal{B}(z, h)$ are accumulated for a specific testing point $z \in \mathcal{X}$ and bandwidth $h > 0$, the estimate $\widehat{\theta}_n$ and subsequently $\widehat{m}_n(z)$ or $\widehat{f}_n(z)$ can be computed in $O(D^3)$ time and $O(D^2)$ space via Eq. (5), both treated as constants under fixed-dimension (d) settings.

Thus, the computational question reduces to efficient computation of sufficient statistics for every testing point z and bandwidth h .² To simplify our presentation, we abstract the sufficient statistics as

$$\mathcal{T}_\ell^{z, h} = \sum_{\mathcal{B}(z, h)} T_\ell(X_i, Y_i), \quad \ell = 1, 2, \dots, M, \quad (6)$$

² In this paper we consider constant bandwidths h for every testing point. Nevertheless, our algorithm framework can be easily modified to handle heterogeneous bandwidths as well.

where M is the total number of sufficient statistics required. A simple brute-force algorithm loops over all $\{(X_i, Y_i)\}_{i=1}^n$ and takes $O(n)$ time to calculate $\mathcal{T}_\ell^{z,h}$ for each testing point z , which results in an overall $O(sn)$ quadratic time complexity. Further optimization of computational procedures of $\mathcal{T}_\ell^{z,h}$ is the focus of the rest of this section.

3.2. The univariate case: a warm-up exercise

Before giving the full description of our algorithm, we first consider the basic univariate case ($d = 1$) and show a simple algorithm that computes $\mathcal{T}_\ell^{z,h}$ for each $z \in \mathcal{X}$ and $h > 0$ in $O(\log n)$ time. Though simple, the univariate algorithm serves as a conceptual starting point for our follow-up development of general high-dimensional algorithms.

Let $\{(X_i, Y_i)\}_{i=1}^n$ be the training data points where $X_i, Y_i \in \mathbb{R}$. As pre-processing steps, (X_i, Y_i) are sorted in ascending order with respect to X_i , such that $X_1 \leq X_2 \leq \dots \leq X_n$, and for each $\ell = 1, \dots, M$ the cumulative statistics

$$\mathcal{A}_\ell(i) = \sum_{j \leq i} T_\ell(X_j, Y_j) \quad i = 1, 2, \dots, n \quad (7)$$

are computed by a sweeping algorithm from $i = 1$ to $i = n$. It is clear that the pre-processing can be done in $O(n \log n + Mn)$ time with $O(Mn)$ space.

Afterwards, for each testing point $z \in \mathbb{R}$ and $h > 0$, the left and right “boundaries” $L = \arg \max\{i : X_i < z - h/2\}$ and $U = \arg \max\{i : X_i \leq z + h/2\}$ are found by binary searches. The sufficient statistic $\mathcal{T}_\ell^{z,h} = \sum_{z-h/2 \leq X_i \leq z+h/2} T_\ell(X_i, Y_i)$ can then be computed as

$$\mathcal{T}_\ell^{z,h} = \mathcal{A}_\ell(U) - \mathcal{A}_\ell(L). \quad (8)$$

The time required to compute $\hat{m}_n(z)$ can then be upper bounded by $O(\log n + M)$. The overall time complexity on s testing points is then $O((n + s)(\log n + M))$, which is simply $O((n + s) \log n)$ because M only depends on d and k , both treated as constants in this paper.

3.3. Discretization in multiple dimensions

The sorting and partial sum idea in Eq. (8) can be formally generalized to multiple dimensions $d > 1$ via the argument of *discretization*. (See the leftmost plot of Figure 2 for a graphical illustration.) Specifically, for each dimension $j \in \{1, \dots, d\}$, the values $X_{1j}, X_{2j}, \dots, X_{nj} \in \mathbb{R}$ are sorted in ascending order. We also denote $\lambda_j(i)$ as the i th smallest value in $\{X_{1j}, \dots, X_{nj}\}$ (repetitions counted as multiple values). By performing such

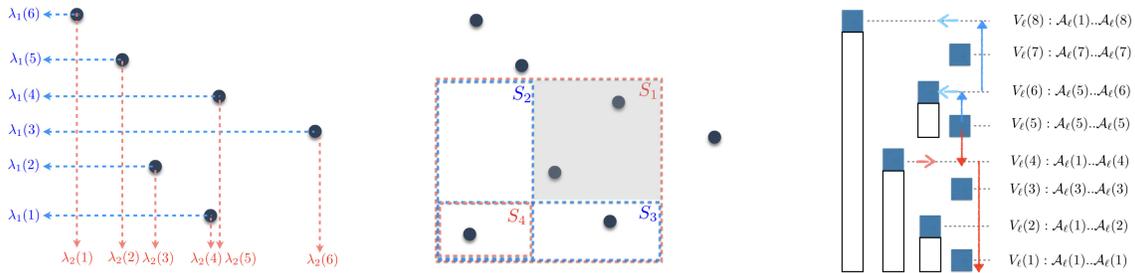


Figure 2 The left figure demonstrates how discretization is carried out when $d=2$, where each of the two dimensions is treated separately and $\lambda_j(1)$ through $\lambda_j(6)$ record the values on a particular dimension $j \in \{1, 2\}$. The middle figure illustrates the inclusion-exclusion principle used to calculate cumulative statistics in the shaded region of interest, by considering $S_1 - S_2 - S_3 + S_4$. The right figure depicts the one-dimensional binary indexed tree structure for a toy example of $n=8$ data points, with each $V_\ell(\cdot)$ indicating over what region is the cumulative statistics supposed to be calculated. The red arrows indicate the interrogation path when $\mathcal{A}_\ell(5)$ is evaluated ($5 \rightarrow 4 \rightarrow 0$), and the blue arrows indicate the update path when $T_\ell(5)$ is added ($5 \rightarrow 6 \rightarrow 8$).

“discretization” on all dimensions, every training point $X_i \in \mathcal{X}$ can be mapped to a unique k -tuple $\chi_i = (\chi_{i1}, \dots, \chi_{id}) \in [n]^d$, where $[n] = \{1, 2, \dots, n\}$.

Similar to the definition of $\mathcal{A}_\ell(i)$ in the $d=1$ setting, for the general multivariate case define

$$\mathcal{A}_\ell(i_1, \dots, i_d) = \sum_{t=1}^n \mathbb{I}[\chi_{t1} \leq i_1, \dots, \chi_{td} \leq i_d] T_\ell(X_t, Y_t)$$

for $i_1, \dots, i_d \in [n]$. Suppose for now that $\mathcal{A}_\ell(i_1, \dots, i_d)$ are available for all ℓ and i_1, \dots, i_d by some pre-processing procedure. To compute the estimate $\hat{m}_n(z)$, first find L_1, \dots, L_d and U_1, \dots, U_d by binary searches, where (for $j=1, \dots, d$)

$$\begin{aligned} L_j &= \arg \max \{i : \lambda_j(i) < z_j - h/2\}; \\ U_j &= \arg \max \{i : \lambda_j(i) \leq z_j + h/2\}. \end{aligned} \quad (9)$$

The sufficient statistics $\mathcal{T}_\ell^{z,h}$ can then be computed as

$$\mathcal{T}_\ell^{z,h} = \sum_{\nu_1, \dots, \nu_d \in \{0,1\}^d} (-1)^{\nu_1 + \dots + \nu_d} \mathcal{A}_\ell(i_1^{(\nu_1)}, \dots, i_d^{(\nu_d)}),$$

where $i_j^{(0)} = U_j$ and $i_j^{(1)} = L_j$. The validity of the computational formula for $\mathcal{T}_\ell^{z,h}$ is implied by the inclusion-exclusion principle, and involves 2^d evaluations of $\mathcal{A}_\ell(i_1, \dots, i_d)$. An illustrative example of the $d=2$ case is given in the middle plot of Figure 2.

The question remains to design fast algorithms that compute $\mathcal{A}_\ell(i_1, \dots, i_d)$ for arbitrary input tuple $(i_1, \dots, i_d) \in [n]^d$. In the basic univariate case of $d=1$, this is accomplished by

a sweeping pre-processing that records $\mathcal{A}_\ell(i)$ for all $i \in [n]$. Such an approach, however, no longer works for $d > 1$ because a sweeping algorithm that records all $\mathcal{A}_\ell(i_1, \dots, i_d)$ takes $O(n^d)$ space and time complexity and is clearly impractical. To overcome this difficulty, we consider a data structure named *binary indexed trees* and show how it can compute every $\mathcal{A}_\ell(i_1, \dots, i_d)$ evaluation in $O(\log^d n)$ time.

3.4. Binary indexed trees

The *binary indexed tree* or *Fenwick's tree*, invented and first documented by Fenwick (1994), is a simple yet powerful data structure that supports fast queries and updates of *partial sums*, corresponding to $\mathcal{A}_\ell(i_1, \dots, i_d)$ defined in this paper.

In the rightmost panel of Figure 2 we give a toy example with $n = 8$ data points and $d = 1$. The $V_\ell(i)$ entries for $i = 1, \dots, n$ are the main data structure kept by the binary indexed tree, each corresponding to the cumulative statistics of data points in a specific interval. To query or interrogate a particular partial sum $\mathcal{A}_\ell(i)$, one starts with i and repeatedly rips off the least significant bit (LSB) in the binary expansion of i and accumulates the entries of V_ℓ on the path. For example, for $i = 5$ the query/interrogation path would be $5 \rightarrow 4 \rightarrow 0$. Formally, the following update rule is applied when interrogating partial sum $\mathcal{A}_\ell(i)$:

$$\mathbf{Interrogation} : i \leftarrow i - \text{LSB}(i). \tag{10}$$

Here $\text{LSB}(i)$ denotes the least significant bit of i in its binary expansion.

To add (update) a data point $^3 T_\ell(i)$ to the binary indexed tree, one has to undo the interrogation path in Eq. (10). It is easy to verify that the following update procedure is an exact mirroring of the interrogation rule in Eq. (10):

$$\mathbf{Update} : i \leftarrow i + \text{LSB}(i + 1). \tag{11}$$

For example, starting with $i = 5$ the updating procedure would take us to $5 \rightarrow 6 \rightarrow 8$, meaning that $V_\ell(5)$, $V_\ell(6)$ and $V_\ell(8)$ are updated with the data entry $T_\ell(5)$ added.

To simplify notations, we write $\text{PATH}^I(i)$ and $\text{PATH}^U(i)$ as the interrogation and update paths starting from i , respectively. For example, $\text{PATH}^I(5) = \{5, 4\}$ and $\text{PATH}^U(5) = \{5, 6, 8\}$ if $n = 8$. It is a simple observation that for any $i \in [n]$, $|\text{PATH}^I(i)|, |\text{PATH}^U(i)| =$

³ Here $T_\ell(i)$ denotes $T_\ell(X, Y)$ for the data tuple (X, Y) that corresponds to the i th position in the sorted data locations. $T_\ell(i_1, \dots, i_d)$ has a similar meaning in higher dimensions.

Input: training set $\{(X_i, Y_i)\}_{i=1}^n$, testing set $\{z_i\}_{i=1}^s$, bandwidth $h > 0$, dimension d , polynomial degree k

Output: local polynomial estimates $\{\widehat{m}_n(z_i)\}_{i=1}^s$ or $\{\widehat{f}_n(z_i)\}_{i=1}^s$

Initialize: hash functions h_1, \dots, h_d and hash tables $\{\mathcal{H}_\ell\}_{\ell=1}^M$;

▷ *pre-processing steps*

Discretization: for every $j \in [d]$ sort $\{X_{ij}\}_{i=1}^n$ in ascending order and label them $\lambda_j(1), \dots, \lambda_j(d)$;

for each $\ell = 1, \dots, M$ and $t = 1, \dots, n$ **do**

 Compute sufficient statistics $T_\ell(X_t, Y_t)$ and find $i_1, \dots, i_d \in [n]$ such that

$\lambda_1(i_1) = X_{t1}, \dots, \lambda_d(i_d) = X_{td}$;

 Compute update paths $\text{PATH}^U(i_1), \dots, \text{PATH}^U(i_d)$ using Eq. (11);

for $i'_1 \in \text{PATH}^U(i_1), i'_2 \in \text{PATH}^U(i_2), \dots, i'_d \in \text{PATH}^U(i_d)$ **do**

 Update: $\mathcal{H}_\ell(H(i'_1, \dots, i'_d)) \leftarrow \mathcal{H}_\ell(H(i'_1, \dots, i'_d)) + T_\ell(X_t, Y_t)$;

end

end

▷ *compute estimates*

for each $t = 1, \dots, s$ **do**

 Find L_1, \dots, L_d and U_1, \dots, U_d defined in Eq. (9) for z_t and h using binary searches;

for each $\ell = 1, \dots, M$ **do**

for $\nu_1, \nu_2, \dots, \nu_d \in \{0, 1\}$ **do**

 Initialize $\mathcal{A}_\ell(i_1^{(\nu_1)}, \dots, i_d^{(\nu_d)}) = 0$, where $i_j^{(0)} = U_j$ and $i_j^{(1)} = L_j$ for $j \in [d]$;

 Compute interrogation paths $\text{PATH}^I(i_1^{(\nu_1)}), \dots, \text{PATH}^I(i_d^{(\nu_d)})$ using Eq. (10);

for $i'_1 \in \text{PATH}^I(i_1^{(\nu_1)}), \dots, i'_d \in \text{PATH}^I(i_d^{(\nu_d)})$ **do**

 Accumulate: $\mathcal{A}_\ell(i_1^{(\nu_1)}, \dots, i_d^{(\nu_d)}) \leftarrow \mathcal{A}_\ell(i_1^{(\nu_1)}, \dots, i_d^{(\nu_d)}) + \mathcal{H}_\ell(H(i'_1, \dots, i'_d))$;

end

end

 Compute $\mathcal{T}_\ell^{z_t, h} = \sum_{\nu_1, \dots, \nu_d} (-1)^{\nu_1 + \dots + \nu_d} \mathcal{A}_\ell(i_1^{(\nu_1)}, \dots, i_d^{(\nu_d)})$, using the inclusion-exclusion principle;

end

 Obtain estimate $\widehat{m}_n(z_t)$ or $\widehat{f}_n(z_t)$ using Eq. (5) and sufficient statistics $\{\mathcal{T}_\ell^{z_t, h}\}_{\ell=1}^L$;

end

Algorithm 1: The main accelerated local polynomial regression algorithm.

$O(\log n)$. Thus, both interrogation and updating operations (for $d = 1$) can be completed in $O(\log n)$ time.

To extend the univariate binary indexed tree to higher dimensions, consider tuple $i_1, \dots, i_d \in [n]^d$ at which interrogation or update is needed. For evaluation of $\mathcal{A}_\ell(i_1, \dots, i_d)$, accumulate all $V_\ell(i'_1, \dots, i'_d)$ such that $i'_1 \in \text{PATH}^I(i_1), i'_2 \in \text{PATH}^I(i_2), \dots, i'_d \in \text{PATH}^I(i_d)$ and add them together. Similarly, when adding a data point $T_\ell(i_1, \dots, i_d)$, consider all $i'_1 \in \text{PATH}^U(i_1), i'_2 \in \text{PATH}^U(i_2), \dots, i'_d \in \text{PATH}^U(i_d)$ and update each $V_\ell(i'_1, \dots, i'_d)$ with $T_\ell(i_1, \dots, i_d)$. The time complexity for both interrogation and updating is $O(\log^d n)$.

3.5. Lazy memory allocation via Hashing

Although the time complexity of d -dimensional binary indexed trees is $O(\log^d n)$ and is small, the space complexity is another story. A naive implementation of the multi-dimensional binary indexed tree would require $O(n^d)$ memory to store all $V_\ell(i_1, \dots, i_d)$ values. It is imperative to design more intelligent space allocation algorithms that significantly reduce the $O(n^d)$ space complexity for practical usages.

An important observation of the multi-dimensional binary indexed tree is that the V_ℓ values are extremely *sparse*, with most of the entries equal to zero. More specifically, with n points in the training data set, the number of non-zero entries of V_ℓ is at most $O(n \log^d n)$ because each data point is associated with a update path of length at most $O(\log^d n)$, which is significantly smaller than $O(n^d)$. This motivates us to consider a *lazy memory allocation* scheme based on Hash tables, which would subsequently reduce the space complexity from $O(n^d)$ to nearly $O(n \log^d n)$.

In particular, we construct M hash tables $\{\mathcal{H}_\ell\}_{\ell=1}^M$ each corresponding to a sufficient statistics \mathcal{T}_ℓ to be maintained. When adding a new data point $T_\ell(i_1, \dots, i_d)$, we insert all entries $i'_1 \in \text{PATH}^U(i_1), \dots, i'_d \in \text{PATH}^U(i_d)$ into the corresponding Hash table \mathcal{H}_ℓ ; similarly when interrogating a point (i_1, \dots, i_d) we read values off all relevant entries $i'_1 \in \text{PATH}^I(i_1), \dots, i'_d \in \text{PATH}^I(i_d)$ from the Hash table \mathcal{H}_ℓ and add them together.

Let $b \in \mathbb{N}$ be a pre-determined capacity parameter of hash tables $\{\mathcal{H}_\ell\}_{\ell=1}^M$ to be constructed, which satisfies $b = \Omega(n \log^d n)$. Let $\tau \in \mathbb{N}$ be another pre-defined integer. Suppose $h_1, \dots, h_d : [n] \rightarrow [b]$ are τd -wise independent hash functions, meaning that for all $j = 1, \dots, d$ and any $i_1, i_2, \dots, i_{\tau d} \in [n], a_1, \dots, a_{\tau d} \in [b]$,

$$\Pr[h_j(i_1) = a_1 \wedge \dots \wedge h_j(i_{\tau d}) = a_{\tau d}] = b^{-\tau d}.$$

A “composite” hash function $H : [n]^d \rightarrow [b]$ can then be defined as

$$H(i_1, \dots, i_d) := (\hbar_1(i_1) + \dots + \hbar_d(i_d)) \pmod{b}.$$

It is a well-known result that H is a τ -wise independent hash function on $[n]^d$ (see for example (Pham and Pagh 2013, Wang et al. 2015)). The corresponding entry of $(i_1, \dots, i_d) \in [n]^d$ in the Hash table \mathcal{H}_ℓ can then be located at

$$\mathcal{H}_\ell(H(i_1, \dots, i_d)).$$

When collision occurs, standard methods such as *hash chains* or *linear probing* can be employed to resolve collision. In particular, when $\tau = 5$ for linear probing, the expected number of collision would be at a constant level (Pagh et al. 2009, Thorup and Zhang 2012).

3.6. Summary of time and space complexity

The capacity of the Hash table constructed in the previous section, b , can be set as $b \asymp n \log^d n$, leading to the expected number of collision to be upper bounded at a constant level. Hence, the space complexity of the proposed algorithm is $O(n \log^d n)$.

For the time complexity, note that each insertion of a data point $x_i, i \in [n]$ requires M update steps along the update paths in Eq. (11), and each estimate requires $2^d M$ interrogation steps along the interrogation paths in Eq. (10). Because $M \leq (2k)^d + k^d$ and the length of each update/interrogation path is upper bounded by $O(\log^d n)$, the total time complexity of Algorithm 1 is upper bounded by $O((2k)^d(n+s) \log^d n) = O((n+s) \log^d n)$, where both k and d are treated as constants.

4. Numerical results

In this section we use simulations to verify the effectiveness of our proposed algorithm. All source codes of our implementation are provided in the supplementary materials accompanying this paper. The raw data and results in the plotted figures and tables are also provided in a separate online supplement.

We implement algorithm 1 using C++. All simulations are done on a computer installed with Ubuntu 14.04 LTS 64bit OS, 31.4 Gib Memory, Intel Core i7-4970 CPU @3.60GHz x 8, except for the running time reported for our own implementation of the brute-force algorithm which is experimented on a MacBook Pro laptop with macOS Mojave 10.14.6,

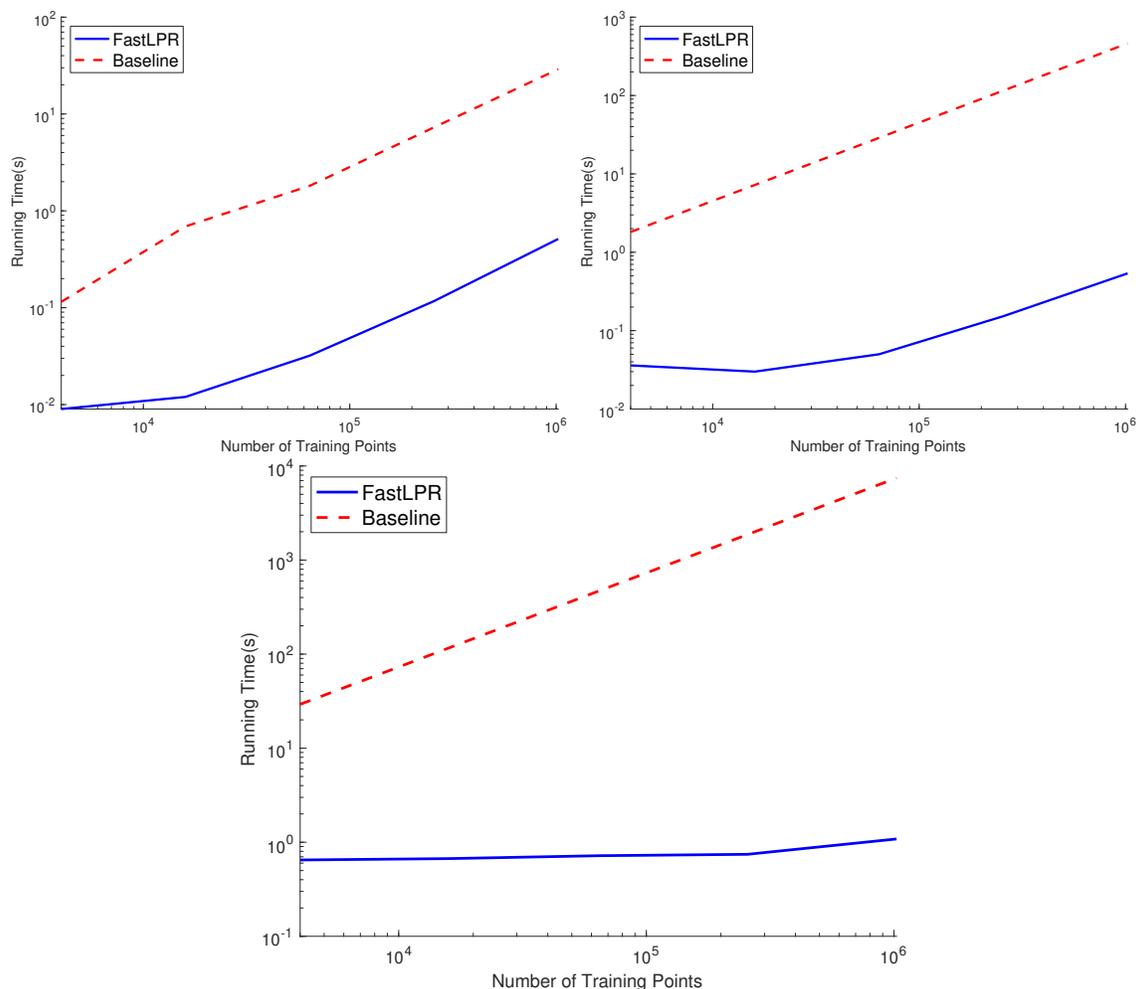


Figure 3 Running times (secs) of fast and baseline implementation of local mean averaging ($k = 0$) for univariate data ($d = 1$), with varying number of testing points $s = 4000$ (left), $s = 64000$ (middle) and $s = 1024000$ (right).

16GB memory, 2.3 GHz Intel Core i9 because the former server has been de-serviced at the time this part of the experiment is carried out.

Two baselines are considered and compared against our proposed method. The first baseline is a widely used R library `locpol`⁴, which is implemented in C. A detailed description of the `locpol` package can be found in (Cabrera 2012). The relevant routines in `locpol` include `locCteSmootherC`, `locLinSmootherC`, `locCuadSmootherC` and `locPolSmootherC`, corresponding to local polynomial estimation of $k = 0$, $k = 1$, $k = 2$ and $k > 2$, respectively. Note that for $d \geq 2$ only local constant regression (i.e., $k = 0$) is supported in `locpol`. While the detailed implementation strategy of `locpol` is not available, judging from the high

⁴ <https://cran.r-project.org/web/packages/locpol>

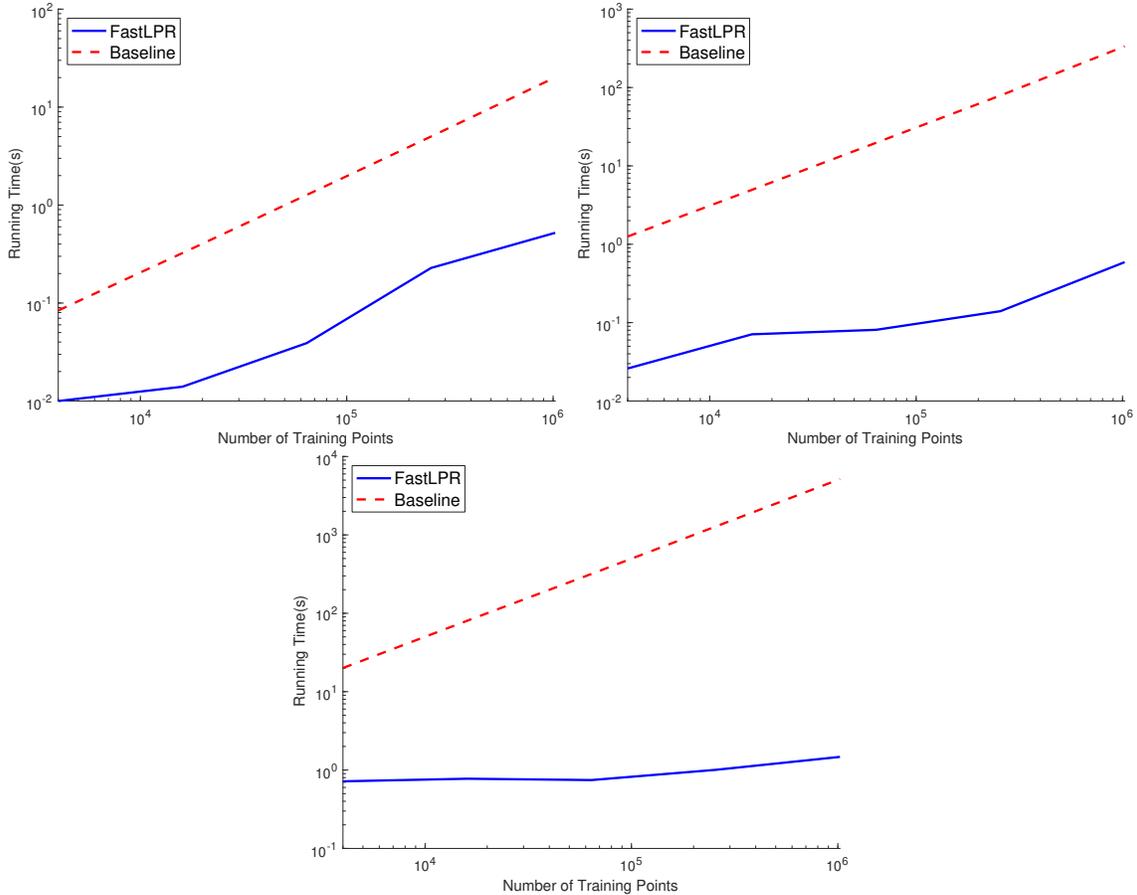


Figure 4 Running times (secs) of fast and baseline implementation of local linear regression ($k = 1$) for univariate data ($d = 1$), with varying number of testing points $s = 4000$ (left), $s = 64000$ (middle) and $s = 1024000$ (right).

computational costs in numerical experiments we conjecture that the naive brute-force implementation is used which computes $\hat{\theta}_n$ separately for each data point.

The second baseline is our own implementation of the brute-force computation of local polynomial estimates, which serves as a second baseline for comparison. We implement the brute-force approach using C++, which supports general data dimension d and polynomial degree k .

We first compare the running times of our fast local polynomial regression implementation (Algorithm 1, denoted as `FastLPR`) with the baseline R package `locpol` under various simulation settings in Figure 3 ($d = 1, k = 0$), Figure 4 ($d = 1, k = 1$) and Figure 5 ($d = 2, k = 0$). The ground-truth functions $f : \mathbb{R}^d \rightarrow \mathbb{R}$ are defined as $f(x_1, \dots, x_d) = \sum_{i=1}^d \sin(x_i)$. Note that for $d = 2$ we only experiment with local mean averaging ($k = 0$) because the `locpol` package only supports $k = 0$ for $d > 1$. For all experimental setups, the running times are

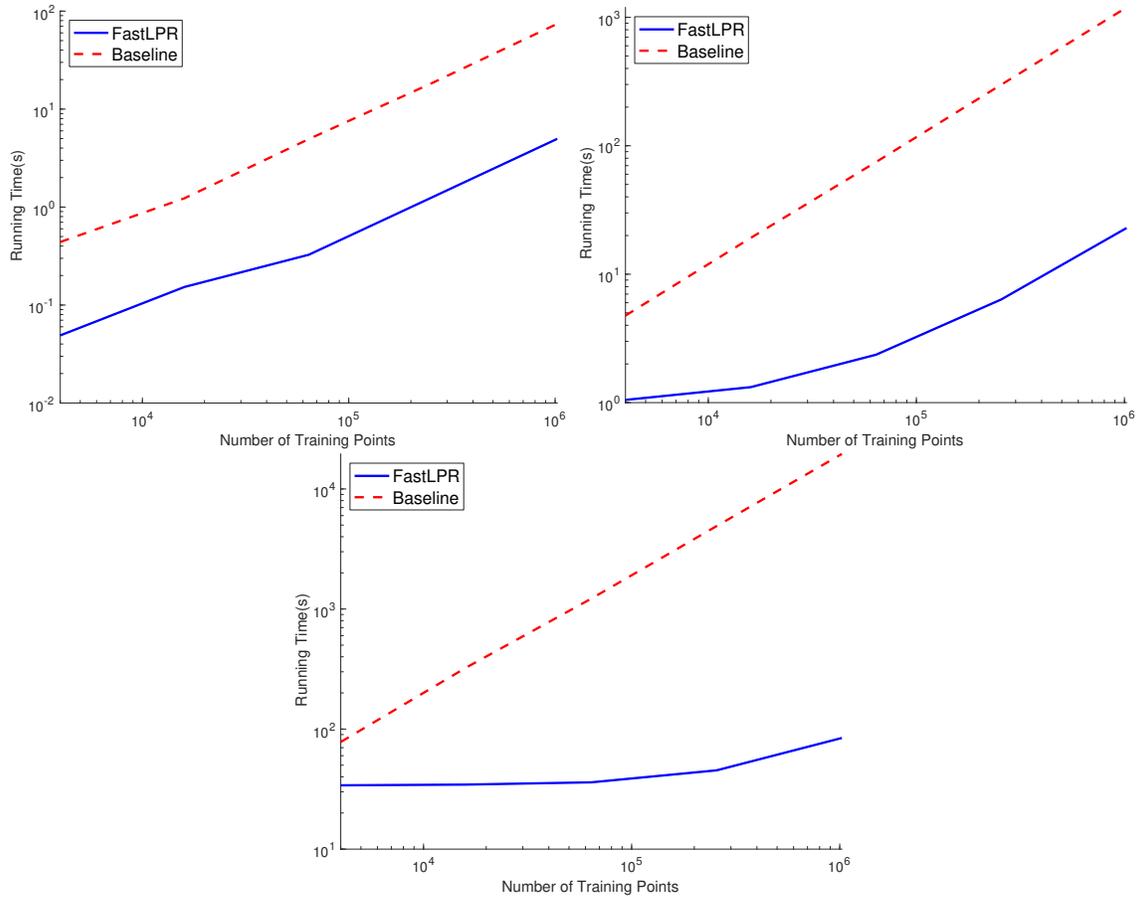


Figure 5 Running times (secs) of fast and baseline implementation of local mean averaging ($k = 0$) for bivariate data ($d = 2$), with varying number of testing points $s = 4000$ (left), $s = 64000$ (middle) and $s = 1024000$ (right).

reported under varying number of training and testing points, all uniformly sampled from the unit cube $[0, 1]^d$.

From Figures 3, 4 and 5, we observe that as the number of testing points (s) or the training points become larger, the advantages of our proposed algorithm are more significant. In particular, when 1,024,000 training and testing points are present under the setting of $k = 1$ and $d = 1$, Algorithm 1 achieves $40,000\times$ speed-up over the naive implementation in `locpol`. The reason is that the naive implementation has $\Theta(ns)$ time complexity whereas ours is $O((n + s) \log^d n)$.

We compare our algorithm with a baseline implementation of local polynomial regression in Figures 6, 7, 8 on 3-dimensional data (i.e., $d = 3$) with polynomial degrees ranging from $k = 0$ to $k = 2$. Because the `locpol` package in R only supports $k = 0$ for $d > 1$, we compare our proposed algorithm with our own brute-force implementation of local polynomial regression in C++. As we can observe from the figures, our proposed algorithm

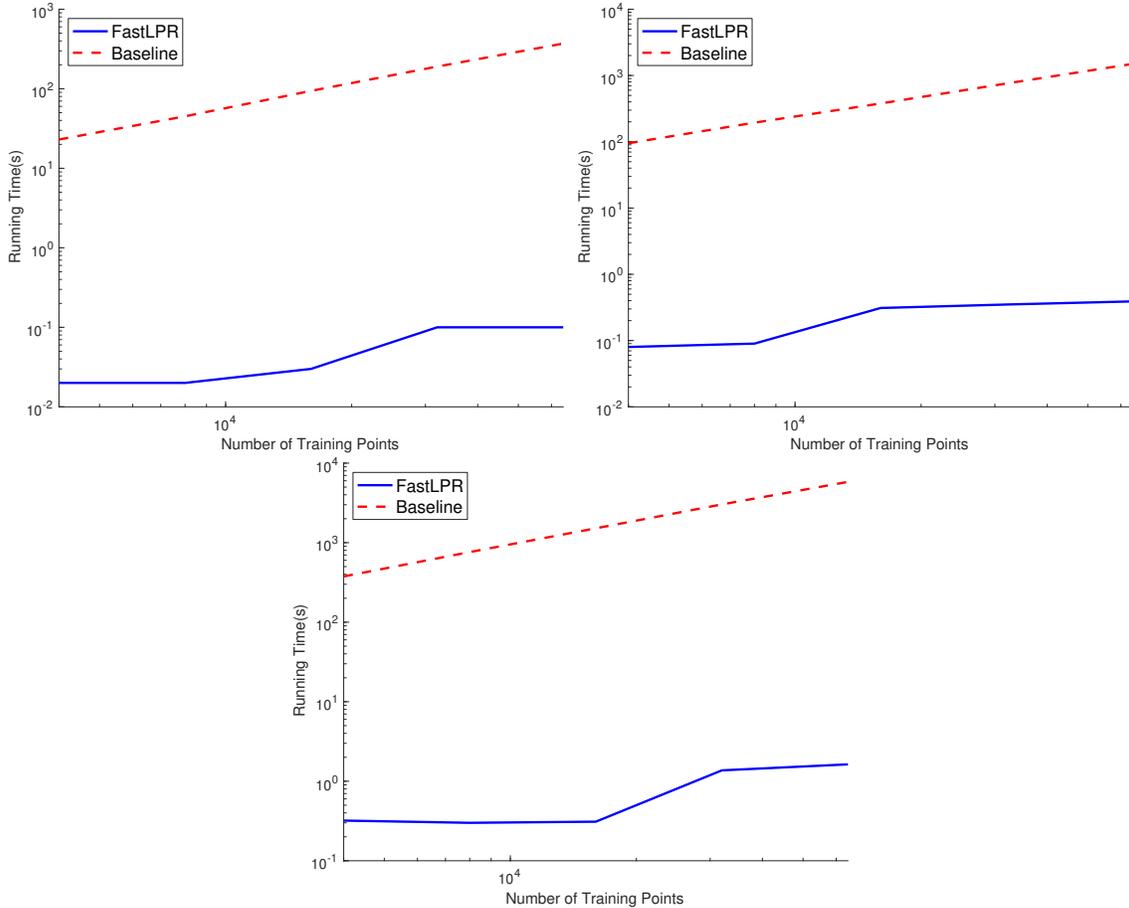


Figure 6 Running times (secs) of fast and baseline implementation of local mean averaging ($k = 0$) for bivariate data ($d = 3$), with varying number of testing points $s = 4000$ (left), $s = 16000$ (middle) and $s = 64000$ (right).

still consistently outperforms the baseline implementation for all polynomial degrees in the case of $d = 3$.

We also compare memory consumptions between our method and the naive method in Table 1. For all experiments we fix $d = 3$ and $s = 4000$ (we found different s do not affect the memory consumption of both methods by much). As we can observe from Table 1, our implementation consumes significantly more memory compared to baseline because the multi-dimensional binary indexed trees is quite a memory-intensive data structure, even with lazy memory allocation schemes in place. Nevertheless, the highest amount of memory consumption (approximately 7GB for $d = 3$, $k = 2$ and $n = 64,000$) is still well within the limit of modern main memories on desktop or workspace computers. Such memory consumption is worthy because of the significant improvement in running time our proposed algorithm brings.

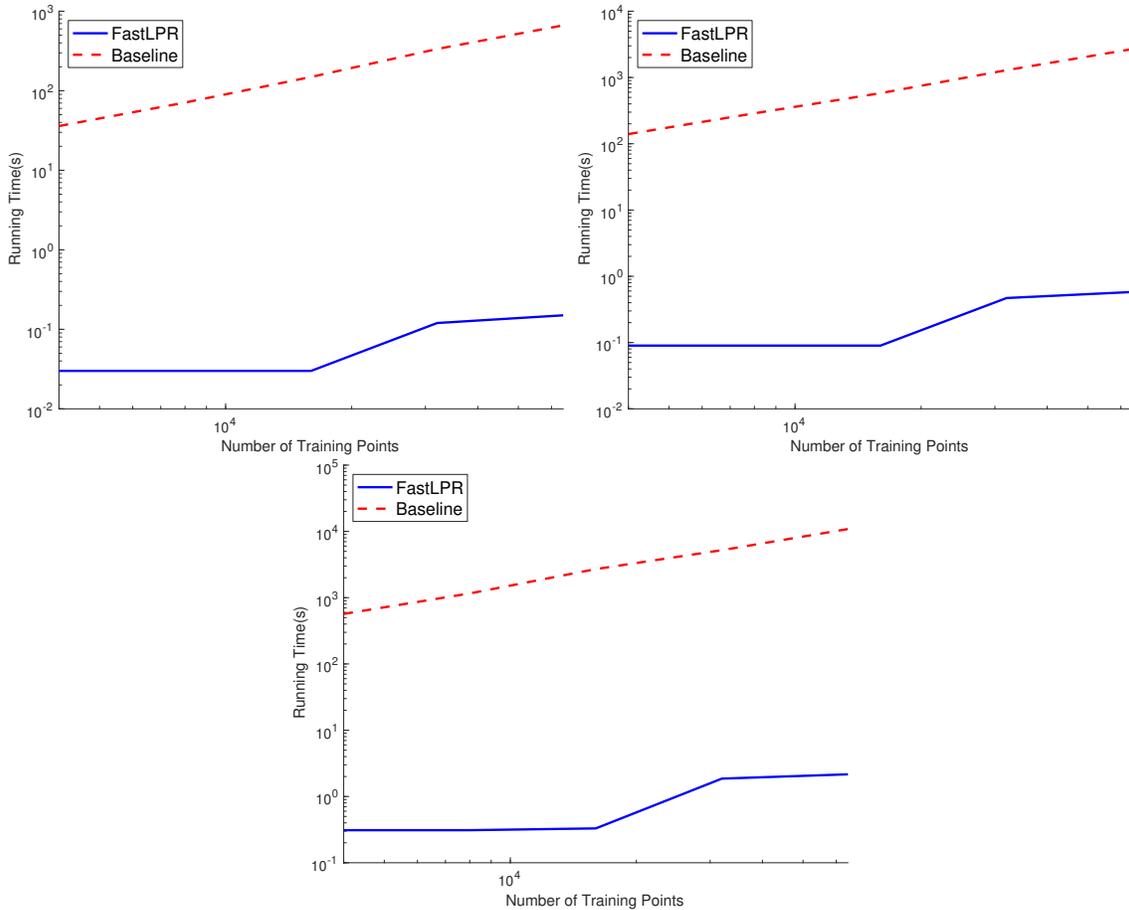


Figure 7 Running times (secs) of fast and baseline implementation of local mean averaging ($k = 1$) for bivariate data ($d = 3$), with varying number of testing points $s = 4000$ (left), $s = 16000$ (middle) and $s = 64000$ (right).

Lastly, we report in Figure 9 the function reconstruction errors of both FastLPR and the baseline method in `locpol` under fixed running time budgets. We fix number of testing points to be 4000 and the bandwidth parameter h takes values of $n^{-1/3}$, $n^{-1/4}$ and $n^{-1/5}$. Figure 9 shows under given time budgets, our proposed FastLPR algorithm processes much more observations (training samples) and therefore achieves significantly smaller reconstruction error.

5. Discussion

Kernel functions. In our accelerated local polynomial estimation algorithm, the kernel $K(\cdot)$ is assumed to be the box kernel $K(u) = \mathbb{I}[|u| \leq 1/2]$ and for multiple dimensions ($d \geq 2$) the “composite kernel” is defined in terms of ℓ_∞ norm, meaning that the kernel evaluation between $x, z \in \mathbb{R}^d$ is $K(\|x - z\|_\infty/h)$. The box kernel ensures that the sufficient statistics can be expressed as a linear combination of unweighted partial sums, and the ℓ_∞

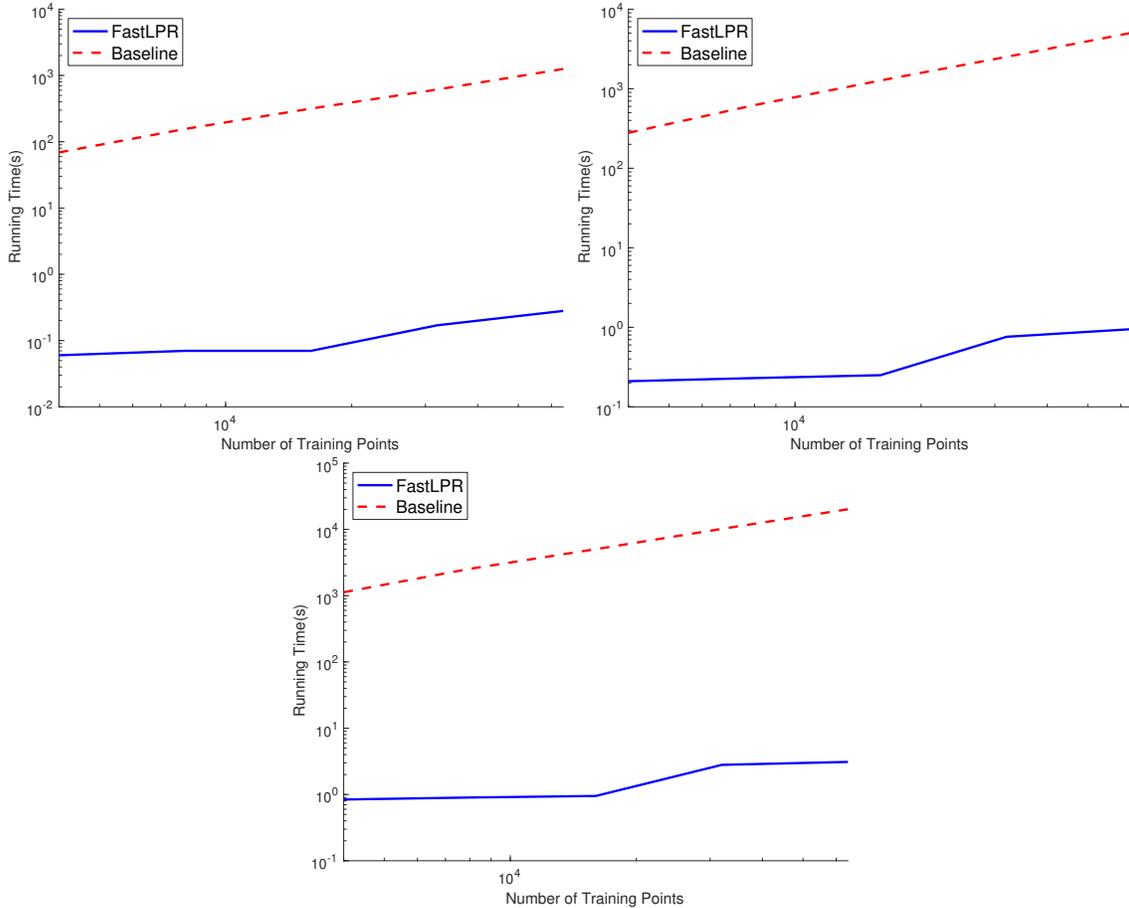


Figure 8 Running times (secs) of fast and baseline implementation of local mean averaging ($k = 2$) for bivariate data ($d = 3$), with varying number of testing points $s = 4000$ (left), $s = 16000$ (middle) and $s = 64000$ (right).

norm in multi-variate kernel evaluations lead to rectangle regions whose edges are parallel to the standard basis. Both properties are crucial for our algorithmic development that enables fast sufficient statistics computation via binary indexed trees.

In general, box kernels with ℓ_∞ distance measures are sufficient as they achieve the same minimax statistical efficiency as other kernel functions and/or equivalent distance measures. However, for certain applications it might be desirable to consider kernel functions *smoother* than the box kernel (e.g., the Gaussian kernel $K(u) = e^{-u^2/2}/\sqrt{2\pi}$) to obtain smoother function fits. We believe significantly different techniques are required to handle such kernels that are non-uniform and not restricted to parallel rectangular neighborhoods of testing points.

Incremental training and testing sets. While in the description of our algorithm the sizes of both training and testing sets (n and s) are fixed a priori, we remark that our algorithm can perfectly handle training and testing data with increasing sizes. In particular,

	Our implementation (MB)	Baseline (MB)
$k = 0, n = 4000$	72	1.3
$k = 0, n = 8000$	170	1.4
$k = 0, n = 16000$	432	2.3
$k = 0, n = 32000$	1044	3.7
$k = 0, n = 64000$	2485	6.3
$k = 1, n = 4000$	73	1.3
$k = 1, n = 8000$	181	1.6
$k = 1, n = 16000$	443	2.5
$k = 1, n = 32000$	2221	3.9
$k = 1, n = 64000$	4945	6.6
$k = 2, n = 4000$	354	4.2
$k = 2, n = 8000$	897	8.5
$k = 2, n = 16000$	2217	16.5
$k = 2, n = 32000$	5280	28.4
$k = 2, n = 64000$	7642	52.8

Table 1 Comparison of memory consumption between our method and the naive method. For all experiments we fix $d = 3$ and $s = 4000$.

for every new training or testing point, the corresponding update or interrogation paths are calculated in $O(\log^d n)$ time and the Hash tables can be updated/queried using a similar amount of running time. This property is particularly useful in applications where training data constantly grow/change, and estimates on incoming test points have to be made in a real-time fashion.

Further acceleration with approximate computation. In cases where exact computations of local polynomial estimates are not mandatory and small error in the estimates can be tolerated, it is possible to further reduce the time and space complexity beyond $O(n \log^d n)$.

One approach is to consider significantly smaller (shorter) Hash tables with capacity $b \ll n \log^d n$. Because the capacity of Hash tables is significantly smaller than the number of entries created by binary indexed trees, collisions are unavoidable. Instead of resolving

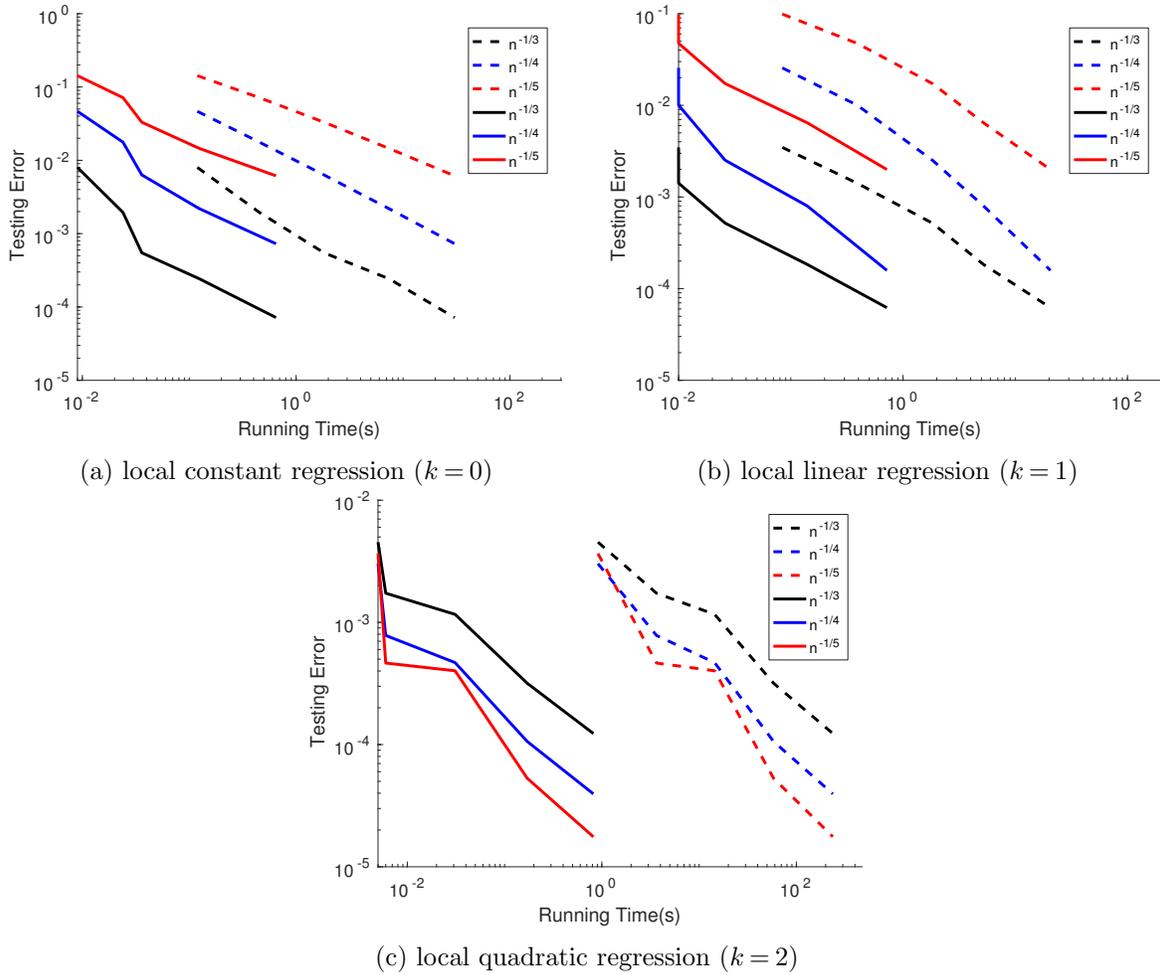


Figure 9 Local polynomial regression for one dimensional data with running time constraints. Solid lines correspond to FastLPR and dot lines correspond to BaseLine.

collisions completely, one can borrow the ideas of COUNTSKETCH (Charikar et al. 2004) that multiplies an additional Rademacher variable ⁵ $\sigma(i_1, \dots, i_d)$ in Hash table updates:

$$\begin{aligned} \mathcal{H}_\ell(H(i_1, \dots, i_d)) &\leftarrow \mathcal{H}_\ell(H(i_1, \dots, i_d)) \\ &+ \sigma(i_1, \dots, i_d)T_\ell(i_1, \dots, i_d). \end{aligned}$$

Dependency on data dimension d . The time complexity of our proposed algorithm has a leading $O((2k)^d)$ term which scales exponentially with data dimension d , which is dropped in the main $O((n + s) \log^d n)$ time complexity bound because both polynomial degree k and data dimension d are treated as constants in this paper. On the other hand, the naive approach has an $O(n^2)$ time complexity and does not explicitly depend exponentially on

⁵ A Rademacher random variable takes on values of ± 1 with equal probability.

d. Nevertheless, in nonparametric regression/estimation it is typical that an exponential number of sample points are required (e.g., to estimate a Lipschitz continuous function up to precision ε , $\Omega(\varepsilon^{-(2+d)})$ samples are needed (Tsybakov 2009)). Hence, our $O((n+s)\log^d n)$ time complexity is generally much more preferable than the $O(n^2)$ time complexity of naive approaches.

6. Conclusion

In this paper we propose nearly linear time algorithms that compute local polynomial estimates for nonparametric density and regression function estimates. Our algorithm is based on the novel application of multivariate binary indexed trees together with discretization and hashing techniques. Simulation results demonstrate an up to $40000\times$ speed-up over state-of-the-art R implementation of local polynomial regression. Future directions including general kernel functions and further algorithmic acceleration via sketching approximation are discussed.

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