Density Estimation on a Network

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Abstract

This paper develops a novel approach to density estimation on a network. We formulate nonparametric density estimation on a network as a nonparametric regression problem by binning. Nonparametric regression using local polynomial kernel-weighted least squares have been studied rigorously [Ruppert and Wand (1994)], and its asymptotic properties make it superior to kernel estimators such as the Nadaraya-Waston estimator. Often, there are no compelling reasons to assume that a density will be continuous at a vertex and real examples suggest that densities often are discontinuous at vertices. To estimate the density in a neighborhood of a vertex, we propose a two-step local piecewise polynomial regression procedure. The first step of this pretest estimator fits a separate local polynomial regression on each edge using data only on that edge, and then tests for equality of the estimates at the vertex. If the null hypothesis is not rejected, then the second step re-estimates the regression function in a small neighborhood of the vertex, subject to a joint equality constraint. Since the derivative of the density may be discontinuous at the vertex, we propose a piecewise polynomial local regression estimate. We study in detail the special case of local piecewise linear regression and derive the leading bias and variance terms using weighted least squares matrix theory. We show that the proposed approach will remove the bias near a vertex that has been noted for existing methods.

Keywords: Asymptotic bias and variance, discontinuous density, kernel density estimation, local piecewise linear estimation, pretest estimation

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1 Introduction

In this paper, we analyze spatial patterns of points that lie on a network. There are numerous types of events that can occur along networks. The lines or curves that form the network may be roads, rivers, subway lines, airline routes, electrical wires, or nerve fibers. The events may be vehicles, street crimes, car accidents, retail stores, or neuroanatomical features such as dendritic spines. For a recent summary of applications that involve the modelling of point patterns on a network of lines, see Baddeley et al. (2015). In order to carry out analyses of those events, researchers need a range of specific techniques.

One of the frequently demanded tasks is density estimation on a network, but few statistical methods had been developed to address this need until recently. A natural first attempt at analyzing such data is to take the kernel density estimate (KDE) on the one-dimensional real line

$$\hat{f}(x) = \frac{1}{N} \sum_{i=1}^{N} K_h(x_i - x),$$

and translate it directly to the linear network by defining $x_i - x$ as the network distance, where $x$ is any location on the network, and $x_1, \ldots, x_N$ are the observed data locations. The problem with this approach is that it does not conserve mass: the induced kernel $K_h(\cdot, x_i)$ is not a probability density on the linear network, and so the estimate (1) is not a probability density. The true probability density will be grossly overestimated in the denser parts of the network. Okabe et al. Okabe and Sugihara (2012) summarized widely used methods for density estimation on a network. Although many published papers, such as Xie and Yan (2008), mentioned by Okabe et al. claim to have computed a kernel density estimate on a network, most appear to have used (1).

There is currently no general agreement on how to perform density estimation on a linear network, and a rigorous foundation is lacking. The two most popular heuristic techniques, namely the equal-split discontinuous kernel estimator and the equal-split continuous kernel estimator (Okabe et al. (2009), Okabe and Sugihara (2012), Sugihara et al. (2010)) give plausible results in applications, but their properties are not well understood, statistical insight is lacking, and computational cost is high. These methods does not allow for discontinuity at vertices, which is found in many applications, such as traffic network, and the example in Figure 1 and Section 7.4. It is also noted that
the equal-split continuous and discontinuous kernel estimator algorithms effectively traverse every path in the network. As the bandwidth $h$ increases, the number of paths and the computation time should increase roughly exponentially.

McSwiggan et al’s approach (McSwiggan et al. 2017) uses the connection between kernel smoothing and diffusion (Botev et al. 2010). On a network, the appropriate counterpart of the Gaussian kernel is the heat kernel. The connection with diffusion provides a sound statistical rationale and helps establish many good theoretical properties. These authors also develop an algorithm that is faster than equal-split continuous/ discontinuous kernel density estimators for density estimation, based on numerical solution of the heat equation. Their method is mathematically equivalent to an infinite-sum generalization of the equal-split continuous kernel density estimation applied to the Gaussian density, and it is asymptotically unbiased with rate $h^2$ away from the boundary region, where $h$ is the bandwidth. At a terminal vertex, it has the standard boundary rate $h$ of KDE. Moreover, similar to previous kernel methods, diffusion approach does not allow for discontinuity at vertices.

In this paper, we take a different approach. We study local piecewise linear regression on a network. It is known that nonparametric density estimation can be formulated as a nonparametric regression problem by binning. The advantage of local polynomial estimation is reduction of the order of the bias, especially when the evaluation point is near or on the boundary, and, as a practical matter, the amount of computation is reduced. By binning, we form a histogram of observations (bin centers and counts) on the network, which is then smoothed by local polynomial regression. The proposed method is not only useful for density estimation, but also nonparametric regression analysis on linear network. To accommodate densities with discontinuous derivatives at vertices, we introduce piecewise linear local regression. As far as we know, local polynomial regression on linear network has not be proposed and investigated and piecewise local linear regression is also new.

To motivate our research and illustrate its contribution to reduce bias at vertices, we introduce the dendrite data collected by the Kosik Lab, UC Santa Barbara, and first analyzed by Baddeley.
et al. (2014) and Jammalamadaka et al. (2013). In this example, the events are dendritic splines, which are of clinical importance. Cognitive disorders such as ADHD and autism may result from abnormalities in dendritic spines, especially the number of spines and their maturity Penzes et al. (2011). The events on the network are the locations of 566 spines observed on one branch of the dendritic tree of a rat neuron, as shown in Figure 1. The density of spines shows clear discontinuity at vertices A, C and D; see Figure 6. We will need a density estimation method that allows for multiple levels of smoothness at vertices – discontinuous, continuous with discontinuous derivative, and continuous with continuous derivative. We show that our proposed method will remove the bias that has been noted for existing methods such as Okabe and Sugihara (2012) and McSwiggan et al. (2017) due to their inflexibility at vertices. In fact, estimation at vertices is a major contribution of this paper.

![Figure 1: Dendritic spines on a branch of the dendrite network of a neuron.](image)

The paper is organized as follows. Section 2 gives basic definitions. In Section 3, a binned local polynomial regression estimator is constructed individually on each edge, and asymptotic properties of the estimator are established. As the evaluation point approaches the vertex from each edge, we obtain limits of the regression functions. In Section 4 we construct an asymptotic test
for the equality of those limits. If the null hypothesis is not rejected, then the regression function
is re-estimated for evaluation points that are within the $h$-neighborhood of a vertex by binned
local piecewise polynomial regression using data from all neighboring edges. These estimators are
constructed and their asymptotic properties are studied in Section 5. In Section 6, we discuss
networks with loops and related computational issues when the bandwidth is large. In Section 7,
we demonstrate the workings of the proposed method with simulated data and a real example.
We end with a discussion in Section 8.

2 Preliminaries

In this section, we introduce basic definitions.

2.1 Network

A segment or edge with vertices $u$ and $v$ is defined as the image of an injective differentiable
function $e : [0, 1] \rightarrow \mathbb{R}^d$ where $e(0) = u$ and $e(1) = v$, so, in the definition of segment, we allow
curved lines. A network $L$ is the union $L = \bigcup_{i=1}^{n} e_i$ of segments (edges) $e_1, \ldots, e_n$ in $\mathbb{R}^d$ where
$1 < n < \infty$. The total length of all segments in $L$ is denoted by $|L|$. The degree $d(v)$ of a vertex $v$
is the number of segments with an endpoints at $v$. A vertex is terminal if it has degree 1. Often,
the network is embedded in a two-dimensional space, such as a street network (if there are no
overpasses). However all of our results generalize easily to a network of curves embedded in a
higher dimensional space, such as the dendrites which are embedded in $R^3$.

A path between two points $x$ and $y$ along $L$ is a sequence $\pi = (x, v_1, \ldots, v_n, y)$, where $v_1, \ldots, v_n$
are vertices, such that $e_j = [v_j, v_{j+1}]$ is an edge of $L$ for each $j = 1, \ldots, n - 1$, while $x$ and $v_1$
lie on a common edge $e_0$, and $y$ and $v_n$ lie on a common edge $e_n$. The path length is
Length($\pi$) = $\int_x^{v_1} |e'_0(t)| dt + \sum_{j=1}^{n-1} \int_{v_j}^{v_{j+1}} |e'_j(t)| dt + \int_{v_n}^{y} |e'_n(t)| dt$, where integration is with respect
to arc length. The shortest path distance $d_L(x, y)$ between $x$ and $y$ in $L$ is the minimum of the
lengths of all paths from $u$ to $v$. If there are no paths from $x$ to $y$, then we define $d_L(x, y) = \infty$.
In the case where there are multiple paths between two points, we will use the shortest path.
2.2 Density and intensity

Suppose that events were observed at locations \( x_1, \ldots, x_n \) on a linear network \( L \). The objective is to estimate the probability density \( f(x) \) from which the locations are assumed to be drawn. The density satisfies \( f(x) \geq 0 \) for all \( x \in L \), and \( \int_L f(x)dx = 1 \). The probability that a random point \( X_i \) with density \( f \) falls in a subset \( B \subseteq L \) is \( P(X_i \in B) = \int_B f(x)dx \).

Equivalently \( x = \{x_1, \ldots, x_n\} \) is a realization of a point process \( X \) on the network, and the objective is to estimate the intensity function \( \lambda(x) \) of \( X \). The intensity is defined so that the number \( N(X \cap B) \) of points of \( X \) falling in \( B \subseteq L \) is Poisson distributed with expectation \( E\{N(X \cap B)\} = \int_B \lambda(u)du \). Stated differently, \( \lambda(u) \) is the expected number of random points per unit length of network in the small neighborhood of \( u \). Estimation of \( f \) and of \( \lambda \) are essentially equivalent because, if \( N \) is fixed, \( \lambda(x) = Nf(x) \) for all locations \( x \in L \).

2.3 Problem statement

In this paper, we consider density estimation via local polynomial regression. This is achieved by way of binning. Here we use the “simple binning” discussed in Hall and Wand (1996). For \( i = 1, \ldots, n \), \( x_i \) are the bin centers, \( c_i \) are bin counts, \( y_i \) are bin heights, and \( \omega \) is bin width. Letting \( N \) be the total number of observations on the linear network, we have \( y_i = c_i/N\omega \). These rectangles form a histogram with total area 1, since the area of the \( i \)th bin is \( c_i/N \) and \( \sum_{i=1}^{n} c_i/N = 1 \). For a chosen \( \omega \), we consider the regression model \( y_i = m(x_i) + \epsilon(x_i) \). We have

\[
E(y_i|x_i) = E\left(\frac{c_i}{N\omega}\right) = \frac{1}{\omega}E(\hat{p}_i) = \frac{1}{\omega}p_i \approx m(x_i),
\]

where \( p_i \) is the expected proportion of points in bin \( i \) for bin width \( \omega \), and \( m(\cdot) \) is the regression function. For the variance, \( \hat{p}_i = c_i/N \) is the sample proportion so

\[
Var(y_i|x_i) = Var\left(\frac{c_i}{N\omega}\right) = \frac{1}{\omega^2}Var(\hat{p}_i) = \frac{p_i - \hat{p}_i^2}{N\omega^2} \approx \frac{1}{N\omega}m(x_i).
\]

The approximate equality symbol is due to the fact that binning introduces a bias, but it can be made negligible for small enough bin width. Hall and Wand studied the accuracy of binned kernel density estimators Hall and Wand (1996), and their results show that, with the commonly-used Epanechnikov kernel, we require \( \omega \) to go to zero faster than \( h \) the bandwidth, if binning is not to
have a significant effect on the bias of the estimator. Therefore, the error term \( \epsilon(x_i) \) has approximately mean zero and variance \( m(x_i)/N\omega \).

Assuming that \( \omega \) is sufficiently small, we can smooth the histogram by local polynomial regression using \((x_i, y_i), i = 1, \ldots, n\), as data. We propose a “pretest” estimation procedure that consists of the following steps:

1. Local polynomial regression on each edge individually.
2. Test joint equality of intercepts at the vertex.
3. If not rejected, then the regression function is re-estimated by local piecewise polynomial regression using data from all neighboring edges for evaluation points that are within the \( h \)-neighborhood of a vertex.

An asymptotic test for joint equality of slopes at the vertex can be constructed similarly.

3 Local polynomial regression

First, we consider each edge individually. This is equivalent to a fixed equally-spaced design model, where the \( x \)-variables are the bin centers \( x_1, \ldots, x_n \), and the \( y \)-variables are the bin heights \( y_1, \ldots, y_n \). We want to estimate the regression function \( m(x) = E(Y|X = x) \). Using a Taylor expansion, we can approximate \( m(x) \), where \( x \) is close to a point \( x_0 \), by a \( p \) degree polynomial:

\[
m(x) \approx m(x_0) + m^{(1)}(x_0)(x - x_0) + \frac{m^{(2)}(x_0)}{2!}(x - x_0)^2 + \cdots + \frac{m^{(p)}(x_0)}{p!}(x - x_0)^p
\]

provided that all the required derivatives exist. The local polynomial regression estimator minimizes with respect to \( \beta_0, \beta_1, \ldots, \beta_p \) the function

\[
\sum_{i=1}^{n} \left\{ y_i - \beta_0 - \beta_1(x_i - x_0) - \cdots - \beta_p(x_i - x_0)^p \right\}^2 K_h(x_i - x_0),
\]

where \( K_h(x_i - x_0) = K(\frac{x_i - x_0}{h})/h \). Let \( \hat{\beta} = \left\{ \hat{\beta}_0, \hat{\beta}_1, \ldots, \hat{\beta}_p \right\} \) denote the minimizer of (2). Then \( \hat{\beta}_0 \) estimates \( m(x) \) and \( s!\hat{\beta}_s \) estimates \( m^{(s)}(x) \), the \( s \)th derivative of \( m(x) \), for \( s = 1, \ldots, p \). Conveniently, (2) is a standard weighted least squares regression problem. Let \( W = \text{diag}\left\{ K_h(x_1 - \right. \}
\]
Define
\[ Y = \begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix}, \quad \text{and} \quad X = \begin{bmatrix} 1 & x_1 - x & \ldots & (x_1 - x)^p \\ \vdots & \vdots & & \vdots \\ 1 & x_n - x & \ldots & (x_n - x)^p \end{bmatrix}. \]

Assuming invertibility of \( X'WX \), then \( \hat{\beta} = (X'WX)^{-1} X'WY \). The estimate of the regression function at \( x \) is \( \hat{m}(x) = \hat{\beta}_0 = e_1^T \hat{\beta} \), where \( e \) is the \((p+1) \times 1\) vector with 1 being the first entry and zero elsewhere. Ruppert and Wand [Ruppert and Wand 1994] studied the leading conditional bias and variance of the above estimator, but here we consider in detail only the local linear \((p = 1)\) binned estimator. We make the following assumptions:

A1 The function \( m^{(2)}(\cdot) \) is continuous.

A2 The kernel \( K \) is symmetric and supported on \((-1, 1)\). Also, \( K \) has a bounded first derivative.

A3 As \( N \to \infty \) and \( \omega \to 0 \), \( Nh \to \infty \) and \( \omega = o(h^2) \), where \( N \) is sample size, \( h \) is bandwidth and \( \omega \) is bin width.

It follows from the definition of the estimator that \( E\{\hat{m}(x)\} \approx e_1^T (X'WX)^{-1} X'WM \), where the vector \( M = \{m(x_1), \ldots, m(x_n)\}^T \) contains the true regression function values at the each of the \( x_i \)'s. For local linear regression we have that
\[
X = \begin{bmatrix} 1 & x_1 - x \\ \vdots & \vdots \\ 1 & x_n - x \end{bmatrix}
\]

Also, \( \text{Var}\{\hat{m}(x)\} = e_1^T (X'WX)^{-1} (X'WVWX) (X'WX)^{-1} e_1 \), where \( V = \text{Var}(Y) \) is a diagonal matrix with diagonal entries \( m(x_i)/\omega N - m(x_i)^2/N \), \( i = 1, \ldots, n \). Note that if \( m \) is a linear function then the local linear estimator is exactly unbiased. To find the leading bias term for general function \( m \), we review the result of local linear regression [Fan 1993] with the binning procedure discussed in [Hall and Wand 1996]. This estimator uses only data on a single edge.
Theorem 1. Suppose that $x$ is a point on the line segment of interest, and that $A1, A2$ and $A3$ hold. Let $\hat{m}(x) = e_i^T (X^T W X)^{-1} X^T W Y$, then

$$E \{ \hat{m}(x) - m(x) \} = \frac{1}{2} h^2 \left\{ \frac{(\sigma_2^2)^2}{\sigma_2^2 - (\sigma_1^2)^2} - \frac{(\sigma_3^2)^2}{\sigma_3^2 - (\sigma_1^2)^2} \right\} m^{(2)}(x) + O(\omega) + o(h^2)$$
\numbered{(4)}

$$\text{Var} \{ \hat{m}(x) \} = C(N, h, \omega, x) Q_K + o \left( \frac{1}{Nh} \right),$$
\numbered{(5)}

where $\sigma_i^2_K = \int u^i K(u) du$, $R_i^K = \int u^i K(u)^2 du$,

$$C(N, h, \omega, x) = \frac{1}{Nh} m(x) + \frac{\omega}{Nh} m(x)^2 \quad \text{and} \quad Q_K = \frac{R_0^K (\sigma_2^2)^2 - 2R_1^K \sigma_2^2 \sigma_1^1 + R_2^K (\sigma_1^1)^2}{\left\{ \sigma_2^2 - (\sigma_1^2)^2 \right\}^2}.$$  \numbered{(6)}

For an interior point $x$, we can simplify (4) and (5). Note that $\sigma_i^2_K = 0$ for odd $i$, we have

$$E \{ \hat{m}(x) - m(x) \} = \frac{1}{2} h^2 \sigma_2^2 m^{(2)}(x) + O(\omega) + o(h^2)$$
\numbered{(7)}

$$\text{Var} \{ \hat{m}(x) \} = C(N, h, \omega, x) R_0^K \quad + o \left( \frac{1}{Nh} \right).$$
\numbered{(8)}

The estimator has the following asymptotic distribution:

$$\hat{m}(x) - m(x) \sim \frac{1}{2} h^2 \left\{ \frac{(\sigma_2^2)^2}{\sigma_2^2 - (\sigma_1^2)^2} - \frac{(\sigma_3^2)^2}{\sigma_3^2 - (\sigma_1^2)^2} \right\} m^{(2)}(x) \quad \overset{d}{\rightarrow} \quad N \{0, C(N, h, \omega, x) Q_K \}.$$
\numbered{(9)}

The local linear estimator has better properties at the boundary than the kernel density estimator. Asymptotically, the local linear estimator’s bias is of the same order at a boundary point as at an interior point. Even if $x$ is at the boundary of the density’s support, since the local linear estimator fits a weighted least squares line through data near the boundary, if the true relationship is linear, this estimator will be exactly unbiased.

Extension to higher order $p$ is straightforward, see Ruppert and Wand (1994). For $p$ odd, the bias is of order $h^{p+1}$ everywhere. When $p$ is even, the bias is of order $h^{p+2}$ away from the boundary but $h^{p+1}$ in the boundary region. By increasing the polynomial order from even to the next odd number, the order of the bias in the interior remains unchanged, but the bias simplifies. On the other hand, by increasing the polynomial order from odd to the next even number, the bias order increases in the interior. This effect is analogous to the bias reduction achieved by higher-order kernels.
4 Test for joint equality at vertex

When multiple edges meet at a vertex, for example a simple network consisting of three edges \(e_1, e_2\) and \(e_3\) and a vertex \(v\) (see Figure 2), there are three estimates for \(m(v)\). One estimate is \(\hat{m}_{e_1}(v)\), the local linear regression estimate of \(m_{e_1}(v) := \lim_{x \to v, x \in e_1} m(x)\) using only data on \(e_1\). The estimates \(\hat{m}_{e_2}(v)\) and \(\hat{m}_{e_3}(v)\) are constructed similarly. In this way, for a vertex connecting \(J\) edges, we obtain \(J\) estimates at that vertex. In this section, we construct a test to study whether the \(m_{e_j}(v)\) for \(j = 1, \ldots, J\) (or any subset) are equal.

Let \(v\) be a vertex and let \(e_l, l = 1, \ldots, J\), be the edges connected by \(v\). We want to test

\[
H_0 : m_{e_1}(x) = m_{e_2}(x) = \cdots = m_{e_J}(x) \tag{10}
\]

\[
H_1 : \text{Not } H_0. \tag{11}
\]

**Theorem 2.** Let \(\hat{m} = \{\hat{m}_{e_1}(v), \ldots, \hat{m}_{e_J}(v)\}^T\), and \(C\) be a contrast matrix such that \(C1 = 0\). Under the null hypothesis, we have

\[
(C\hat{m})^T \Sigma^{-1} C\hat{m} \overset{\alpha}{\sim} \chi^2_{J-1}, \tag{12}
\]

where \(\Sigma = C \text{diag}(V_{e_1}, \ldots, V_{e_J}) C^T\), and \(V_{e_l}\) is the asymptotic variance of the \(i\)th estimator. Here \(\overset{\alpha}{\sim}\) denotes “asymptotically distributed as.”

We note that the test statistic (12) is invariant under the choice of contrast matrices. This is easy to see by noticing that the rows of \(C\) are linearly independent.

5 Estimation with equal intercepts at the vertex

If \(H_0\) is not rejected, then evaluation points within the \(h\)-neighborhood of the vertex can be estimated using data from all neighboring edges, subject to \(m_{e_1}(v) = \cdots = m_{e_J}(v)\). The resulting estimator has a lower variance compared to estimating separately on each edge.

For now, we make the following assumptions:

B1 No loop shorter than \(2h\) in the network.

B2 All edges are longer than \(h\).
If the $h$ neighborhood of the evaluation point $x$ is completely covered by an edge, then the estimator is the same as if we only use data from that edge, and its asymptotic bias and variance are given in Theorem 1. Next, we derive the estimator when the $h$ neighborhood $x$ contains a vertex. Note that, by assumption B1, there is a unique path between the evaluation point and any data point that is within its $h$-neighborhood, and by assumption B2, we only consider the case where the neighborhood of $x$ contains exactly one vertex. For a fixed network, the above assumptions eventually will hold as $N \to \infty$ and $h \to 0$. We will consider the effect of these assumptions on the implementation of the proposed estimator in Section 6.

We note that our estimator will have an additional bias when the test in Section 4 makes a type II error, that is, when the density is not continuous at the vertex but the test accepts that it is continuous. We will investigate this problem in Section 7.3.

5.1 Deriving the estimator

Let us first consider the simple network in Figure 2 and consider a point $x \in e_1$ in the $h$-neighborhood of the vertex $v$, and data points $(x_1, y_1)$ on $e_1$, $(x_2, y_2)$ on $e_2$ and $(x_3, y_3)$ on $e_3$.

![Figure 2: Simple Linear Network.](image)

Using a Taylor expansion up to first order, we can approximate the regression function on $e_1$ at $x_1$ as $m_{e_1}(x_1) \approx m_{e_1}(x) + m_{e_1}^{(1)}(x)(x_1 - x)$ provided that all the required derivatives exist. For the
regression function on $e_2$ at $x_2$, we have

$$m_{e_2}(x_2) \approx m_{e_2}(v) + m_{e_2}^{(1)}(x)(x_2 - v)$$

$$= m_{e_1}(v) + m_{e_2}^{(1)}(x)(x_2 - v)$$

$$\approx m_{e_1}(x) + m_{e_2}^{(1)}(x)(v - x) + m_{e_2}(v)(x_2 - v), \quad (13)$$

where (13) holds because that the regression functions from all edges are assumed to be equal at the vertex, (14) is a Taylor expansion of $m_{e_1}(v)$ at $x$ on $e_1$, and $m_{e_2}^{(1)}(v)$ is defined as $\lim_{x \to v, x \in e_2} m_{e_2}(x)$. Similarly we have

$$m_{e_3}(x_3) \approx m_{e_1}(x) + m_{e_1}^{(1)}(x)(v - x) + m_{e_3}(v)(x_3 - v).$$

For a simple network with one vertex $v$ of degree $J$ and an evaluation point $x$ on $e_1$, we have for $x_i \in e_j$, $j = 1, \ldots, J$ and $j \neq l$, $m_{e_j}(x_i) \approx m_{e_l}(x) + m_{e_l}^{(1)}(x)(v - x) + m_{e_j}(v)(x_i - v)$, and for $x_i \in e_l$, $m_{e_l}(x_i) \approx m_{e_l}(x) + m_{e_l}^{(1)}(x)(x_i - x)$.

Under the above construction, the regression functions agree at the vertex but can have different slopes there. Letting $\beta_0 = m_{e_l}(x)$, $\beta_1(e_l) = m_{e_l}^{(1)}(x)$, and $\beta_1(e_j) = m_{e_j}^{(1)}(v)$ for $j \neq l$, these parameters are estimated by minimizing:

$$\sum_{x_d \in e_l} \{ y_d - \beta_0 + \beta_1(e_l)(x_d - x) \}^2 K_{il} + \sum_{j \neq l} \sum_{x_{ij} \in e_j} \{ y_{ij} - \beta_0 - \beta_1(e_l)(v - x) + \beta_1(e_j)(x_{ij} - v) \}^2 K_{ij},$$

where $K_{ij} = K(d_{ij}/h)$, and $d_{ij}$ is the network distance, i.e., the arc length, between $x_{ij}$ and $x$. In matrix notation, we have

$$(Y - X\beta)^T W (Y - X\beta), \quad (15)$$

where $\beta = [\beta_0, \beta_1(e_1), \ldots, \beta_1(e_J)]^T$ and $X$ is a $n \times (J + 1)$ matrix. The first column of $X$ is identically 1. In the $j$th column, for $j > 1$ and $j \neq l$, the $1 + \sum_{i=1}^{j-1} n_i$ to $\sum_{i=1}^{j} n_i$ entries are \{\(x_{ij} - v\)\}_{i=1, \ldots, n_j}$, where $n_i$ is the number of bin centers on edge $i$, and the remaining entries are zero. In the $l$th column of $X$, the $1 + \sum_{i=1}^{l-1} n_i$ to $\sum_{i=1}^{l} n_i$ entries are \{\(x_d - v\)\}_{i=1, \ldots, n_l}$, and the remaining entries are $v - x$. We also note that $Y = \{y_{ij}\}_{i=1, \ldots, n_j; j=1, \ldots, J}$, and $W = \text{diag}(K_{ij})_{i=1, \ldots, n_j; j=1, \ldots, J}$. 

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The solution to the minimization problem (15) is 
\[ \hat{\beta} = (X^T W X)^{-1} X^T W Y, \]
and the estimate for the regression function at \( x \) under the constraint \( m_{e_1}(v) = \cdots = m_{e_j}(v) \) is given by
\[ \hat{m}(x) = e_1^T (X^T W X)^{-1} X^T W Y. \] (16)

Note that we can extend the above derivation to quadratic and higher order approximation, allowing different \( m_{e_j}(v) \) for all \( j \) under the constraint that \( m_{e_j}' \) are equal for \( p' < p \).

5.2 Asymptotic properties – the local linear case \((p = 1)\)

In this subsection, we make the following assumptions:

C1 The functions \( m_{e_j}(v) \) are equal for all \( j \).

C2 The function \( m_{e_j}^{(2)}(\cdot) \) for all \( j \) are continuous on \( e_j \), excluding the vertex.

C3 The kernel \( K \) is symmetric and supported on \((-1, 1)\). Also, \( K \) has a bounded first derivative.

C4 The vertex \( v \) is always in the \( h \)-neighborhood of \( x \) as \( h \) approaches 0, so \( x \) must approach \( v \) at least as fast as \( h \) approaches 0.

C5 As \( N \to \infty \) and \( \omega \to 0 \), \( Nh \to \infty \) and \( \omega = o(h^2) \), where \( N \) is sample size, \( h \) is bandwidth, and \( \omega \) is bin width.

Note that if C4 does not hold, then we are in the case already studied by Ruppert and Wand \textsuperscript{15}.

**Theorem 3.** Suppose that \( x \in e_1 \) is within the \( h \)-neighborhood of a vertex that connects \( J \) segments, and that C1, C2, C3, C4 and C5 hold. Let \( \hat{m}(x) = e_1^T (X^T W X)^{-1} X^T W Y \), where the matrices are defined as above, then
\[ E \{ \hat{m}(x) - m(x) \} = \frac{1}{2} e_1^T U_0^{-1} \left\{ h^2 R_0 + h(v - x) (R_1 - U_1 U_0^{-1} R_0) \right\} + o(h(v - x)) + o(h^2) + O(\omega), \]
and
\[ \text{Var}(\hat{m}(x)) = C(N, h, \omega, x)e_1^T U_0^{-1} \left[ M_0 + \left( \frac{v - x}{h} \right) (M_0 U_0^{-1} U_1 + M_1 - U_1 U_0^{-1} M_0) \right] U_0^{-1} e_1 \]
\[ + o \left( \frac{1}{Nh} \right) + o \left( \frac{\omega}{Nh^2} \right) + o \left( \frac{v - x}{Nh^2} \right) + o \left( \frac{\omega(v - x)}{Nh^2} \right), \]
where the matrices are defined as follows:
1. \( C(N, h, \omega, x) = (1/Nh)m(x) - (\omega/Nh)m(x)^2 \).

2. \( U_0 \) is symmetric, and its first row is \( \sum_j \mu_0^{(j)} \), \( \mu_1^{(1)} \), \( \ldots, \mu_1^{(J)} \) and its diagonal is \( \sum_j \mu_0^{(j)} \), \( \mu_2^{(1)} \), \( \ldots, \mu_2^{(J)} \), where \( \mu_i^{(j)} = \int_{x_j} u^j K(u) du \). All other entries are zero.

3. \( U_1 \) is symmetric, and its first row is \( 0, -\mu_0^{(1)}, \ldots, -\mu_0^{(l-1)}, \sum_{j \neq l} \mu_0^{(j)}, -\mu_0^{(l+1)}, \ldots, -\mu_0^{(J)} \). Its \((l+1)\)th row is \( \sum_j \mu_0^{(j)}, \mu_1^{(1)}, \ldots, \mu_1^{(l-1)}, 0, \mu_1^{(l+1)}, \ldots, \mu_1^{(J)} \) and its diagonal is \( 0, -2\mu_1^{(1)}, \ldots, -2\mu_1^{(l-1)}, 0, -2\mu_1^{(l+1)}, \ldots, -2\mu_1^{(J)} \). All other entries of \( U_1 \) are zero.

4. \( R_0 \) is a column vector, its first entry is \( \sum_j m_{e_j}^{(2)}(v)\mu_2^{(j)} + m_{e_i}^{(2)}(x)\mu_2^{(i)} \), and the rest are \( m_{e_j}^{(2)}(v)\mu_3^{(j)} \), for \( j = 1, \ldots, J \).

5. \( R_1 \) is a column vector, its first entry is \( -2\sum_j m_{e_j}^{(2)}(v)\mu_1^{(j)} \), and the rest, except the \((l+1)\)th entry, are \( -3m_{e_j}^{(2)}(v)\mu_2^{(j)} \), for \( j \neq l + 1 \), and the \((l+1)\)th entry is \( \sum_j m_{e_j}^{(2)}(x)\mu_2^{(j)} \), for \( j = l + 1 \).

6. \( M_0 \) is symmetric, its first row is \( \sum_j R_0^{(j)}, R_1^{(1)}, \ldots, R_1^{(J)} \), and its diagonal entries are \( \sum_j R_0^{(j)}, R_2^{(1)}, \ldots, R_2^{(J)} \). All the other entries of \( M_0 \) are zero.

7. \( M_1 \) is symmetric, its first row is \( 0, -R_0^{(1)}, \ldots, -R_0^{(l-1)}, \sum_j R_0^{(j)}, -R_0^{(l+1)}, \ldots, -R_0^{(J)} \), its \((l+1)\)th row is \( \sum_j R_0^{(j)}, R_1^{(1)}, \ldots, R_1^{(l-1)}, 0, R_1^{(l+1)}, \ldots, R_1^{(J)} \), and its diagonal is \( 0, -R_1^{(1)}, \ldots, -R_1^{(l-1)}, 0, -R_1^{(l+1)}, \ldots, -R_1^{(J)} \). All other entries of \( M_1 \) are zero.

Note that for \( v \) to be in the \( h \)-neighborhood of the evaluation point \( x \), we need \( v - x < h \), and for \( v \) to stay in the \( h \)-neighborhood of the evaluation point asymptotically, we need \( x \) to approach \( v \) at least as fast as \( h \) approaches 0. So \( (v - x)/h \) is small and approaches zero as \( N \to \infty \).

### 5.3 Estimation with equal first derivatives at the vertex

We have studied the asymptotic properties of local piecewise linear regression estimator at evaluation points that are within the \( h \)-neighborhood of a vertex, under the assumption that \( m_{e_j}(v) \), \( j = 1, \ldots, J \), agree at the vertex. Similarly, we can construct an asymptotic test for the joint equality of the limits of \( m_{e_j}^{(1)}(x) \), \( j = 1, \ldots, J \), as \( x \to v \) along multiple edges. If we accept the null hypothesis that the first derivatives are equal at the vertex, this constraint should be added.
to the estimation procedure. For example, in Figure 2 consider an evaluation point \( x \in e_1 \) and a data point \( x_2 \in e_2 \). Using local linear approximations, we have

\[
m_{e_2}(x_2) \approx m_{e_2}(v) + m_{e_2}^{(1)}(v)(x_2 - v) \\
= m_{e_1}(v) + m_{e_2}^{(1)}(v)(x_2 - v) \\
\approx m_{e_1}(x) + m_{e_1}^{(1)}(x)(v - x) + m_{e_2}^{(1)}(v)(x_2 - v) \\
\approx m_{e_1}(x) + m_{e_1}^{(1)}(x)(v - x) + m_{e_1}^{(1)}(v)(x_2 - v).
\]

(17)

The regression function at \( x_3 \in e_3 \) has a similar expansion. In the last line we used \( m_{e_2}^{(1)}(v) = m_{e_1}^{(1)}(v) \), and expand \( m_{e_1}^{(1)}(v) \) around the evaluation point \( x \) on \( e_1 \). However to estimate first derivatives, one should use at least local quadratic polynomials.

6 Practical Issues

6.1 Estimation with large bandwidth

In this section, we will describe a more complex situation. When there are loops in the network, we use the shortest path between the evaluation point and a data point, and the distance between the points is defined by the shortest path distance. When there are multiple vertices in the \( h \)-neighborhood of an evaluation point, and vertices have different results from the joint equality tests, we will show that only data points that have direct access to the evaluation point contribute to the estimation. If \( x \) is the evaluation point, \( x_i \) is a data point that is within the \( h \)-neighborhood of \( x \), and \( v_1, \ldots, v_n \) are the vertices on the shortest path between \( x \) and \( x_i \), we say that \( x_i \) has direct access to \( x \) if the \( H_0 \) (Theorem 2) is accepted at all \( v_i, i = 1, \ldots, n \). We will demonstrate this via the following example.
Here $x$ is the evaluation point, and $x_1$, $x_2$ and $x_3$ are data points on edges $e_1$, $e_2$ and $e_3$ respectively. We consider two scenarios:

1. $H_0$ is accepted at $v_1$ and $v_2$,

2. $H_0$ is accepted at $v_1$ and rejected at $v_2$.

In the first scenario, by Taylor expansions, we have

$$m_{e_1}(x_1) \approx m_{e_1}(x) + (x_1 - x)m_{e_1}^{(1)}(x) \tag{18}$$
$$m_{e_2}(x_2) \approx m_{e_2}(v_1) + (x_2 - v_1)m_{e_2}^{(1)}(v_1) \tag{19}$$
$$m_{e_3}(x_3) \approx m_{e_3}(v_2) + (x_3 - v_2)m_{e_3}^{(1)}(v_2). \tag{20}$$

Now, since $H_0$ is accepted at $v_1$ and $v_2$, we have $m_{e_1}(v_1) = m_{e_2}(v_1)$ and $m_{e_3}(v_2) = m_{e_3}(v_2)$, and (19) and (20) become

$$m_{e_2}(x_2) \approx m_{e_1}(x) + (v_1 - x)m_{e_1}^{(1)}(x) + (x_2 - v_1)m_{e_2}^{(1)}(v_1) + (x_3 - v_2)m_{e_3}^{(1)}(v_2) \tag{21}$$

The problem of minimizing $\sum_{i,j} \{y_{ij} - m_{e_j}(x_i)\}^2K_{ij}$ can be set up in the same way as before. However, in the second scenario, since we do not have $m_{e_2}(v_2) = m_{e_3}(v_2)$, the problem becomes minimization of $\sum_{i,j=1,2} \{y_{ij} - m_{e_j}(x_i)\}^2K_{ij} + \sum_{i} \{y_{i3} - m_{e_3}(x_i)\}^2K_{i3}$. We see that the estimation of $m_{e_1}(x)$ only depends on the first summation. In other words, only data points that have direct access to the evaluation point contribute to the estimation of $m(x)$.

### 6.2 Bin width

For fixed sample size, we will let the bin width $\omega \to 0$. For simplicity, we show how this affects the calculation of $(\omega X^TWX)^{-1}\omega X^TWY$. In the case where the regression function is estimated on each edge individually, when $\omega \to 0$, to calculate $\omega X^TWX$ for $x$ near the vertex, we use that the Riemann sum converges to the integral as $\omega \to 0$:

$$\omega \sum_{i=1}^{n} (x_i - x)^pK_h(x_i - x) \to \int_{L} u^pK(u)du = \mu^p(c),$$

16
where \( x = ch \), \( 0 \leq c \leq 1 \), and \( p^p(c) = \int_{-c}^{1-c} u^pK(u)du \) is the \( p \)th truncated moment. Note that when the evaluation point is the vertex itself, \( c = 0 \). The calculation of the term \( \omega X^T W Y \) requires

\[
\omega \sum_{i=1}^{n} y_i(x_i - x)^pK_h(x_i - x) = \sum_{i=1}^{n} \frac{c_i}{N}(x_i - x)^pK_h(x_i - x) \to \frac{1}{N} \sum_{i=1}^{N} (z_i - x)^pK_h(z_i - x).
\]

Here \( y \) is bar height and \( \omega \) is bar width, so \( y\omega \) is bar area, which equals to \( c/N \), where \( c \) is bar count and \( N \) is sample size. Let \( z_i \) be the location of \( i \)th observation. As \( \omega \to 0 \), eventually each bin is either empty or has exactly one observation in it. Therefore bin count \( c_i \) is 0 for most bins, and 1 for bins that contain one observation, and the location of that observation becomes the bin center in the limit.

When the joint equality constraint is added, to approximate \( \omega X^T W X \) for \( x \in e_l \) near the vertex, we also need to calculate, for \( j \neq l \), \( x_{ij} \in e_j \),

\[
\omega \sum_{i=1}^{n} (x_{ij} - v)K_h(x_{ij} - x) \to h\mu^1(c) - (v - x)\mu^0(c)
\]

\[
\omega \sum_{i=1}^{n} (x_{ij} - v)^2K_h(x_{ij} - x) \to h^2_2\mu^2(c) - 2h\mu^1(c) + (v - x)^2\mu^0(c).
\]

Binning with \( \omega \) fixed might still be used with very large sample size.

### 7 Implementation

#### 7.1 Simulation studies

Let us consider the simple network shown in Figure 2. Three edges meet at a vertex. We propose three interesting cases on this network using the beta distribution. The three cases that we report here are

1. We simulate 500 points on each edge, with the vertex being the origin, from \( Beta(1, 2) \), \( Beta(1, 3) \), and \( Beta(1, 4) \) respectively.

2. We simulate 500 points on each edge, with the vertex being the origin, from \( Beta(1, 4) \).

3. For each edge, with the vertex being the origin, we simulate 500 points from the truncated (from 0.5 to 1) \( Beta(4, 4) \). Then the points are shifted to the vertex by 0.5 and finally
multiplied by 2, so the support of the true density on each edge is from the vertex to a point that is unit distance away from the vertex.

The true density function over the network is normalized so it integrates to 1. Our simulation study focuses on demonstrating that the proposed estimator can accommodate various behaviors of the true regression function (the true density function), especially at the vertex, namely, discontinuous (Case I), continuous with discontinuous first derivative (Case II), and continuous with continuous first derivative (Case III).

Simulation results for one dataset are shown in Figure 4. The result for local piecewise linear density is presented in the last row. The network is in red, and the true density functions over the network are the black dashed lines. The blue lines are our estimates. The first column is case I, where the joint equality test for the regression functions at the vertex is rejected, and our estimate is equivalent to local linear regression on each edge. The second column is case II. We first fitted a local linear regression model on each edge, and tested joint equality at the vertex. Since we fail to reject the null hypothesis, we re-estimated the regression function in the $h$-neighborhood of $v$ using data from all neighboring edges subject to the equality constraint. Turning to case III in the third column, the estimate is also subject to the joint equality constraint.

In case III, in addition to joint equality of the regression functions at the vertex, joint equality of their first derivatives is also established. For better viewing and comparison between different amounts of smoothness at the vertex, Figure 5 zooms in at the vertex. Estimation in left panel of Figure 5 is subject to only one constraint (joint equality of the regression functions at the vertex). However, after testing, by adding the constraint that the first derivatives are jointly zero, we see in the right panel of Figure 5 that the estimated curve is smoother over the vertex. This is desired because the true density function is continuous and has continuous first derivative over the vertex.

We should note that any sufficiently small bin width will do, but selection of the bandwidth takes more care. Since we have converted the problem to nonparametric regression, cross-validation could be used for bandwidth selection.
7.2 Comparison with existing methods

Let us consider again the three cases described in Section 7.1 and apply the equal-split discontinuous kernel estimator (ESDK) Okabe et al. (2009), the equal-split continuous kernel estimator (ESCK) Okabe and Sugihara (2012), and the diffusion estimator (DE) McSwiggan et al. (2017) to each case.

ESDK Okabe et al. (2009) modifies (1), so it conserves mass. The algorithm makes a copy of the kernel function for each evaluation point, confined to the line edge containing that point. At each fork, the remaining tail of the kernel is split equally between the outgoing edges. Suppose there are $J - 1$ outgoing edges, each outgoing edge receives a copy of the kernel tail weighted by $1/(J - 1)$. ESCK Okabe and Sugihara (2012) uses another modified version of (1). At each fork, with $J - 1$ outgoing edges, each outgoing edge receives a copy of the kernel weighted by $2/J$, while the incoming segment receives a copy with the negative weight $2/J - 1$. DE McSwiggan et al. (2017) uses the estimator $\hat{f}(u) = \sum_{i=1}^{N} K_t(u|x_i)/N$, where $K_t(u|z)$ is the heat kernel on a network Botev et al. (2010). Intuitively, $K_t(u|z)du$ is the probability that a Brownian motion on the network, started at location $z \in L_T$ at time 0, will fall in the infinitesimal interval of length $du$ around the point $u$ at time $t$. The bandwidth parameters for ESDK, ESCK, and DE are selected by cross validation.

Figure 5 illustrates the performances of ESDK, ESCK and DE, compared to LPPR. Columns one, two and three correspond to cases I, II and III, respectively. For case I (discontinuous density), both ESCK and DE produce a continuous estimate at the vertex. ESDK, however, produces a discontinuous estimate, but the bias is still significant. Although ESDK is not a standard kernel density estimator, one should note that the asymptotic bias of kernel density estimation has order of $h$ on the boundary, whereas local linear estimation has order of $h^2$. The significant bias at the vertex can be also due to the fact that ESDK uses data from all neighboring edges as the evaluation point approaches the vertex, so it overestimates low density edges and underestimate high density edges.
For case II (continuous density with discontinuous first derivative), ESDK produces a discontinuous estimate. Although ESCK and DE produce continuous estimates, their bias are considerably higher compared to local piecewise polynomial estimation. This is due to lower order of the asymptotic bias of the kernel estimator near a vertex.

For case III (the density and its first derivative are both continuous) the vertex behaves like an interior point. While ESDK still produces a discontinuous estimate, ESCK and DE are comparable to local piecewise linear estimation, because the asymptotic bias of kernel density estimation and local linear estimation are both of order $h^2$ at an interior point. However, ESCK and DE do not estimate the derivatives of the estimated curves as the evaluation point approaching a vertex from multiple directions. Hence, these methods are inadequate when the derivatives are of interest.

Finally we report the bias, standard deviation, and mean squared error of the proposed local (piecewise) polynomial regression compared to all existing methods. In each case (I, II and III), the result is based on simulation of 100 data sets, and each data set consists of 1000 data points on each edge. Bias, standard deviation and mean squared error are reported at the vertex as it is approached from $e_2$ (see Figure 2). The simulation result is summarised in Table 1. We see that ESDK, ESCK and DE only produce comparable results when the vertex behaves like an interior point, whereas LPPR is superior in all other cases. Simulations are run on a Macbook Pro Mid 2005 with 2.5 GHz Intel Core i7. Average time (Case I, II and III) for LPPR, ESDK, ESCK and DE are 6.0082 secs, 4.3217 hrs, 6.4872 hrs and 6.6266 secs for all 1000 datasets. ESDK, ESCK and DE are implemented in the R package spatstat.

### 7.3 Type II error and additional bias

Our estimator will have an additional bias when the test that the density is continuous at a vertex makes a type II error, that is, when the density is not continuous but the test accepts that it is continuous. We investigate this problem through simulations. For simplicity, let the origin be a vertex, and let the two unit-length edges meet at the vertex. On the left edge, we first sample 1000 points from Beta($1, \beta_l$), then multiply the sample by $-1$, so the data points on the left edge range from $-1$ to $0$. On the right edge, we draw 1000 point from Beta($1, \beta_r$). Pairs of ($\beta_l, \beta_r$) are given in
| Case | Bias  | SD    | MSE  | Bias  | SD    | MSE  | Bias  | SD    | MSE  |
|------|-------|-------|------|-------|-------|------|-------|-------|------|
| I    | -0.0621 | 0.0593 | 0.0074 | -0.0629 | 0.0423 | 0.0057 | -0.0971 | 0.0123 | 0.0096 |
| II   | -0.4481 | 0.0196 | 0.2011 | -0.2711 | 0.0229 | 0.0741 | -0.1062 | 0.0121 | 0.0114 |
| III  | -0.4956 | 0.0184 | 0.2459 | -0.2312 | 0.0301 | 0.0542 | -0.1324 | 0.0100 | 0.0176 |
| DE   | -0.4670 | 0.0172 | 0.2180 | -0.2438 | 0.0173 | 0.0597 | -0.1140 | 0.0116 | 0.0131 |

Table 1: Bias, standard deviation, and mean squared error of the proposed local (piecewise) polynomial regression compared to all existing methods. The result is based on 100 simulations of Cases I, III and III with 1000 data points on each edge. Bias, standard deviation and mean squared error are reported at the vertex as it is approached from $e_2$ in Figure 2.

The first column of Table 2 Type II error rate is the probability that the test (Theorem 2) accepts the null hypothesis that the true density is continuous at a vertex when it is not. We perform 3000 simulations of 1000 data points per edge for each pair of $(\beta_l, \beta_r)$. We report the bias, standard deviation and mean squared error at the vertex approached from the right edge. The result is summarized in Table 2. We see that when type II error rates are large, LPPR under the continuity constraint produces little additional bias due to small gaps between $\beta_l$ and $\beta_r$. Similarly, when $\beta_l$ and $\beta_r$ are far apart, there is also little additional bias due to small type II error rates. On the other hand, when type II error rate is in the mid range, for example from 0.6 to 0.7, there is considerable amount of additional bias at the vertex. Hence in the bias column, we should see bigger (in magnitude) biases in the middle rows, and as we approach the top and bottom rows, biases become smaller (in magnitude). Finally we note that the top row has bigger bias than the bottom row, despite that the type II error rate is practically zero. This is due to that local linear regression generally has bigger bias for functions with greater curvature (Beta(1, 4.5) compared to Beta(1, 4)).

7.4 Application to real data

In this section we apply the proposed local piecewise polynomial regression to dendrite data. The data was collected by the Kosik Lab, UC Santa Barbara, and first analyzed by Baddeley et al. (2014) and Jammalamadaka et al. (2013). Dendrites are branching filaments which extend from
| \((\beta_l, \beta_r)\) | Type II error rate | Bias | SD    | MSE    |
|--------------------|-------------------|------|-------|--------|
| \((3.5, 4.5)\)     | 0.0056            | −0.0796 | 0.1480 | 0.0209 |
| \((3.55, 4.45)\)   | 0.0227            | −0.0786 | 0.1482 | 0.0199 |
| \((3.6, 4.4)\)     | 0.0540            | −0.0811 | 0.1458 | 0.0215 |
| \((3.65, 4.35)\)   | 0.1283            | −0.0833 | 0.1453 | 0.0207 |
| \((3.7, 4.3)\)     | 0.2453            | −0.0861 | 0.1487 | 0.0210 |
| \((3.75, 4.25)\)   | 0.3906            | −0.0925 | 0.1454 | 0.0203 |
| \((3.8, 4.2)\)     | 0.6030            | −0.1017 | 0.1398 | 0.0183 |
| \((3.85, 4.15)\)   | 0.7633            | −0.1040 | 0.1245 | 0.0158 |
| \((3.9, 4.1)\)     | 0.8863            | −0.0956 | 0.1135 | 0.0136 |
| \((3.95, 4.05)\)   | 0.9460            | −0.0781 | 0.1038 | 0.0127 |
| \((4, 4)\)         | NA                | −0.0631 | 0.1013 | 0.0140 |

Table 2: Type II error, bias, standard deviation and mean squared error at the vertex approached from the right edge, based on 3000 simulations of 1000 data points per edge in each scenario.

the main body of a neuron (nerve cell) to propagate electrochemical signals. Spines are small protrusions on the dendrites. The network shown in Figure 1 is one of the ten dendritic trees of this neuron. A dendritic tree consists of all dendrites issuing from a single root branching off the cell body; each neuron typically has 4 to 10 dendritic trees. This example was chosen because it is large enough to demonstrate our techniques clearly, without being too large for graphical purposes. The events on the network are the locations of 566 spines observed on one branch of the dendritic tree of a rat neuron. Figure 6 shows the result of applying the proposed local (piecewise) polynomial estimator to the dendrite data of Figure 1. We show density estimates at vertices A, B, C and D. We used a fixed bandwidth of 8 microns (the network has a total length of 1933.653 microns), and we will leave bandwidth selection and variable bandwidths to future projects. Unlike ESDK, ESCK and DE, the continuity of the LPPR estimates at a vertex is only imposed when there is evidence that the density is continuous there. In this case, LPPR estimates provide strong evidence that the density is not continuous at the vertex.
8 Discussion

As we mentioned in the introduction, there is great potential demand in many fields for estimating the density of events on a network. An easy method for such estimations is to use the ordinary kernel density estimation method that assumes an unbounded plane, or kernel density estimation on the real line with the Euclidean distance replaced by network distance. Many papers in the literature employ this method. However, this method yields a bias in density estimation and so the method is likely to lead to misleading conclusions. We also discussed the equal-split discontinuous kernel estimator, the equal-split continuous kernel estimator, and diffusion estimator. None of those methods allows for discontinuity in the estimates. The first two methods lack theoretical justification and are computationally expensive. The diffusion estimator is mathematically equivalent to an infinite-sum generalization of the equal-split continuous rule applied to the Gaussian density, and it inherits the asymptotic properties of a kernel density estimator. Also the diffusion estimator has a slower rate for the boundary bias.

In this paper, we have formulated a density estimation procedure on a linear network via local piecewise polynomial regression by way of binning. We first apply local polynomial regression on each edge individually, then we test joint equality of the regression functions at the vertex. If the null hypothesis is not rejected, locations within the $h$-neighborhood of the vertex are re-estimated by local piecewise polynomial regression using data from all neighboring edges, subject to the equality constraint. The proposed procedure allows for discontinuity at vertices, and asymptotic bias has the same rate at a vertex as an interior point. We studied the local linear case in detail, while there is a straightforward extension to higher-order polynomial approximation. When applying the proposed method to real data, if there are loops in the network, for simplicity, we only considered the shortest path between points, and we showed that only data points that have direct access to the evaluation point contribute to the estimation of the regression function.

We have only considered only fixed-bandwidth smoothing, and we have not considered data-based bandwidth selection nor adaptive smoothing on a network. We proposed a test of equal intercepts at a vertex to decide whether to assume equal intercepts when estimating the density in the neighborhood of the vertex. In the future, we will consider an estimator that shrinks the
unequal-intercepts estimator towards the equal-intercepts estimator. We have assumed that all
locations are measured without error and lie exactly on the linear network. However this is not
true for some applications, such as ambulance or taxi, where there are GPS error in their loca-
tions. Further study into such measurement error problems is required. In addition to estimating
probability density or point process intensity, the proposed procedure is also used for regression
problems, such as varying coefficient models on a linear network.

9 Proofs

Proof of Theorem 1. By Taylor expansion,

$$E(\hat{m}(x) - m(x)) = e_1^T \omega^{-1} (X^TWX)^{-1} \omega X^TW \frac{1}{2} m^{(2)}(x) \begin{bmatrix} (x_1 - x)^2 \\ \vdots \\ (x_n - x)^2 \end{bmatrix} + \ldots.$$  (22)

Note that if $m$ is a linear function then $m^{(r)}(x) = 0$ for $r \geq 2$ so that the local linear estimator is
exactly unbiased when $m$ is a linear function. To find the leading bias term for general function
$m$, note that

$$\omega X^TWX = \begin{bmatrix} \sigma_{K1}^0 & h\sigma_{K1}^1 \\ h\sigma_{K1}^1 & h^2\sigma_{K2}^2 \end{bmatrix} + O(\omega) \quad \text{and} \quad \omega X^TW \begin{bmatrix} (x_1 - x)^2 \\ \vdots \\ (x_n - x)^2 \end{bmatrix} = \begin{bmatrix} h^2\sigma_{K2}^2 \\ h^3\sigma_{K3}^3 \end{bmatrix} + O(\omega),$$  (23)

where $\sigma_{iK}^j = \int u^iK(u)du$. Some straightforward matrix algebra then leads to the following expres-
sion for the leading bias term

$$E(\hat{m}(x) - m(x)) = \frac{1}{2} h^2 \left[ \frac{(\sigma_{K1}^2 - \sigma_{K2}^2)}{\sigma_{K2}^2 - (\sigma_{K1}^1)^2} \right] m^{(2)}(x) + O(\omega) + o(h^2).$$  (24)

To derive the asymptotic variance of $\hat{m}(x)$ we have

$$Var(\hat{m}(x)) = \omega e_1^T (\omega X^TWX)^{-1} (\omega X^TWWWX) (\omega X^TWX)^{-1} e_1,$$  (25)

where $V = \text{diag}(f(x_1), \ldots, f(x_n))$, with $f(x_i) = (1/N\omega)m(x_i) - (1/N)m(x_i)^2$. We stress that $f(x_i)$
depends on $N$ and $\omega$, but we drop them from its notation for simplicity. Now use approximation
analogous to those used above we have
\[ \omega \left( X^T W V W X \right) = \begin{bmatrix} \frac{1}{h} f(x) R_K^0 + o \left( \frac{1}{h} \right) & f(x) R_K^1 + o(1) & \omega \left( \frac{1}{Nh} \right) \\ f(x) R_K^1 + o(1) & h f(x) R_K^2 + o(h) & \omega \left( \frac{1}{Nh} \right) \end{bmatrix} + O(\omega), \] (26)
where \( R_K^i = \int u^i K(u)^2 du \). These expressions can be combined to obtain
\[ \text{Var} \left( \hat{m}(x) \right) = C(N, h, \omega, x) Q_K + o \left( \frac{1}{Nh} \right) + o \left( \frac{\omega}{Nh} \right), \] (27)
where \( C(N, h, \omega, x) = f(x) \omega / h \), and
\[ Q_K = \frac{R_K^0 (\sigma_K^2)^2 - 2 R_K^1 \sigma_K^2 \sigma_K + R_K^2 (\sigma_K^1)^2}{\left[ \sigma_K^2 - (\sigma_K^1)^2 \right]^2}. \] (28)

**Proof of Theorem 2.** Recall the asymptotic result of local polynomial regression:
\[ \sqrt{nh} [\hat{m}_{e_1}(x) - m_{e_1}(x) - B_{e_1}] \xrightarrow{d} N (0, V_{e_1}), \]
where \( B_{e_1} \) and \( V_{e_1} \) are the asymptotic bias and variance of \( \hat{m}_{e_1}(x) \). Let \( \hat{m} = (\hat{m}_{e_1}(v), \ldots, \hat{m}_{e_J}(v))^T \), we have asymptotically, \( h \to 0 \) and \( nh \to \infty \),
\[ \hat{m} \sim N \left( \begin{bmatrix} m_{e_1}(x) + B_{e_1} \\ \vdots \\ m_{e_J}(x) + B_{e_J} \end{bmatrix}, \begin{bmatrix} V_{e_1} & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & V_{e_J} \end{bmatrix} \right). \]
Now consider a \((J - 1) \times J\) contrast matrix \( C \) such that \( C 1 = 0 \) (i.e. each row sum to zero). One choice of \( C \) is
\[ C = \begin{bmatrix} 1 & -1 & 0 & 0 & \ldots \\ 1 & 0 & -1 & 0 & \ldots \\ 1 & 0 & 0 & -1 & \ldots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{bmatrix}, \]
which simply contrasts edge 1 with edge 2, edge 1 with edge 3. Then
\[ C \hat{m} \sim N (\mu, \Sigma) \]
where

\[ \mu = \begin{bmatrix} m_{e_1}(x) - m_{e_2}(x) + B_{e_1} - B_{e_2} \\ \\ \\ m_{e_1}(x) - m_{e_1}(x) + B_{e_1} - B_{e_1} \end{bmatrix} \quad \text{and} \quad \Sigma = \begin{bmatrix} V_{e_1} + V_{e_2} & \cdots & V_{e_1} \\ \vdots & \ddots & \vdots \\ V_{e_1} & \cdots & V_{e_1} + V_{e_2} \end{bmatrix}. \]

Under the null hypothesis,

\[ C\hat{m} \sim N(0, \Sigma). \]

We want to calculate the probability of generating a point at least as unlikely as the observed data point. To do that, we note that under the null hypothesis, the Mahalanobis distance follows a chi-square distribution

\[ (C\hat{m})^T \Sigma^{-1} C\hat{m} \sim \chi^2_{j-1}. \]

The test statistic is invariant under the choice of contrast matrices. This is easy to see by noticing that the rows of \( C \) are linearly independent. So we have a basis of some vector space \( V \) (and it doesn’t matter if \( V \) is all of \( \mathbb{R}^{p+1} \), or some subspace thereof), and two different ordered bases for \( V, b_1 \) and \( b_2 \) (necessarily of the same size, since two bases of the same vector space always have the same size, here they are the transpose of two contrast matrices \( C_1 \) and \( C_2 \)):

\[ b_1 = [v_1, v_2, \ldots, v_n] \]
\[ b_2 = [w_1, w_2, \ldots, w_n]. \]

A change-of-basis matrix is a matrix that translates from \( b_1 \) coordinates to \( b_2 \) coordinates. That is, \( A \) is a change-of-basis matrix (from \( b_1 \) to \( b_2 \)) if, given the coordinate vector \([x]_{b_1}\) of a vector \( x \) relative to \( b_1 \), then \( A[x]_{b_1} = [x]_{b_2} \) gives the coordinate vector of \( x \) relative to \( b_2 \), for all \( x \) in \( V \).

To get a change-of-basis matrix, we write each vector of \( b_1 \) in terms of \( b_2 \), and these are the columns of \( A \), for \( i = 1, \ldots, n \), \( v_i = a_{i1}w_1 + a_{i2}w_2 + \cdots + a_{in}w_n \). We know we can do this because \( b_2 \) is a basis, so we can express any vector (in particular, the vectors in \( b_1 \)) as linear combinations of the vectors in \( b_2 \). Then the change-of-basis matrix translating from \( b_1 \) to \( b_2 \) is

\[ A = \begin{bmatrix} a_{11} & \cdots & a_{1n} \\ \vdots & \ddots & \vdots \\ a_{n1} & \cdots & a_{nn} \end{bmatrix}. \]
Matrix $A$ is always invertible. This is because just like there is a change-of-basis from $b_1$ to $b_2$, there is also a change-of-basis from $b_2$ to $b_1$. Since $b_1$ is a basis, we can express every vector in $b_2$ using the vectors in $b_1$, for $i = 1, \ldots, n$, $w_i = b_{1i}v_1 + b_{2i}v_2 + \cdots + b_{ni}v_n$. So the matrix $B$, with

\[
B = \begin{bmatrix}
b_{11} & \cdots & b_{1n} \\
\vdots & \ddots & \vdots \\
b_{n1} & \cdots & b_{nn}
\end{bmatrix},
\]

has the property that given any vector $x$, if $[x]_{b_2}$ is the coordinate vector of $x$ relative to $b_2$, then $B[x]_{b_2} = [x]_{b_1}$ is the coordinate vector of $x$ relative to $b_1$. Then applying first $A$ and then $B$ translates $b_1$ coordinates into $b_2$ coordinates and back to $b_1$ coordinates, and thus $AB$ must be the identity matrix (likewise for $BA$). So $A$ and $B$ are both invertible, and every change-of-basis matrix is necessarily invertible.

\textit{Proof of Theorem 3.} Standard calculation shows that the leading term of the bias is given by

\[
\frac{1}{2}e_1^T \omega^{-1} (X^T WX)^{-1} \omega X^T WS,
\]

where $S$ is a column vector with entries being $(v - x)^2 m_{ei}^{(2)}(x) + (x_{ij} - v)^2 m_{ei}^{(2)}(v)$, for $i = 1, \ldots, n_j$, and $j = 1, \ldots, J$. Note that for data points $x_{ij} \in e_l$, where $e_l$ is the edge that the evaluation point $x$ is located, the entries are simplified to $(x_{il} - x)^2 m_{ei}^{(2)}(x)$, for $i = 1, \ldots, n_l$. To approximate $\omega^{-1} (X^T WX)^{-1}$, we note that

\[
\begin{align*}
\omega \sum_i (x_{ij} - v) K_h(x_{ij} - x) &= h \mu_1^{(j)} - (v - x) \mu_0^{(j)} + O(\omega), \\
\omega \sum_i (x_{ij} - v)^2 K_h(x_{ij} - x) &= h^2 \mu_2^{(j)} + (v - x)^2 \mu_0^{(j)} - 2h(v - x) \mu_1^{(j)} - O((v - x)\omega) + O(\omega), \\
\omega \sum_i (x_{il} - x)^p K_h(x_{il} - x) &= h^p \mu_p^{(l)} + O(\omega) \quad \text{for } p = 0, 1, 2,
\end{align*}
\]

where $\mu_i^{(j)} = \int_{e_l} u^i K(u)du$. If follows that

\[
\omega X^T WX = A \left[ U_0 + \left( \frac{v - x}{h} \right) U_1 + \left( \frac{v - x}{h} \right)^2 U_2 \right] A + O(\omega 1),
\]

where $A = \text{diag}(1, h, \ldots, h)$. The matrix $U_0$ is symmetric, and its first row is $\sum_j \mu_0^{(j)}, \mu_1^{(1)}, \ldots, \mu_1^{(J)}$ and its diagonal is $\sum_j \mu_0^{(j)}, \mu_2^{(1)}, \ldots, \mu_2^{(J)}$. All other entries are zero. We also have that matrix
$U_1$ is symmetric, and its first row is 0, $-\mu_0^{(1)}, \ldots, -\mu_0^{(l-1)}, \sum_{j \neq l} \mu_0^{(j)}, -\mu_0^{(l+1)}, \ldots, -\mu_0^{(J)}$. Its $(l + 1)$th row is $\sum_{j \neq l} \mu_0^{(j)}, \mu_1^{(1)}, \ldots, \mu_1^{(l-1)}, 0, \mu_1^{(l+1)}, \ldots, \mu_1^{(J)}$ and its diagonal is 0, $-2\mu_1^{(1)}, \ldots, -2\mu_1^{(l-1)}, 0, -2\mu_1^{(l+1)}, \ldots, -2\mu_1^{(J)}$. All other entries of $U_1$ are zero. Finally $U_2 = diag(0, \mu_0^{(1)}, \ldots, \mu_0^{(J)})$.

Take inverse we have

$$
\omega^{-1} (X^T W X)^{-1} = A^{-1} \left[ U_0^{-1} - \left( \frac{v - x}{h} \right) U_0^{-1} U_1 U_0^{-1} + \left( \frac{v - x}{h} \right)^2 U_0^{-1} U_2 U_0^{-1} \right] A^{-1}
+ o \left( \left( \frac{v - x}{h} \right)^2 A^{-1} A^{-1} \right) + O(\omega A^{-1} A^{-1}).
$$

To approximate $\omega X^T W S$, we note that

$$
\sum_i (x_{ij} - v)^3 m_e(x_j(v) K_h(x_{ij} - x) = h^3 \mu_3^{(j)} - (v - x)^3 \mu_0^{(j)} - 3(v - x)h^2 \mu_2^{(j)} + 3(v - x)^2 h \mu_1^{(j)}
+ O((v - x)\omega) + O((v - x)^2 \omega) + O((v - x)^3 \omega) + O(\omega).
$$

Combining this result with the approximations before, we get

$$
\omega X^T W S = A \left[ h^2 R_0 + h(v - x) R_1 + (v - x)^2 R_2 + \frac{(v - x)^3}{h} R_3 \right] + O(\omega),
$$

where $R_0$, $R_1$, $R_2$ and $R_3$ are column vectors. The first entry of $R_0$ is $\sum_{j \neq l} m_e(x_j(v) \mu_2^{(j)} + m_e(x_l(v) \mu_2^{(l)}$, and the rest are $m_e(x_j(v) \mu_3^{(j)}$, for $j = 1, \ldots, J$. The first entry of $R_1$ is $-2 \sum_{j \neq l} m_e(x_j(v) \mu_1^{(j)}$, and the rest, except the $(l + 1)$th entry, are $-3m_e(x_j(v) \mu_2^{(j)}$, for $j \neq l + 1$, and the $(l + 1)$th entry is $\sum_{j \neq l} m_e(x_j(v) \mu_2^{(j)}$. The first entry of $R_2$ is $m_e(x) \sum_{j \neq l} \mu_0^{(j)} + \sum_{j \neq l} m_e(x) \mu_0^{(j)}$, and the rest, except the $(l + 1)$th entry, are $m_e(x) \mu_1^{(j)} + 3m_e(x) \mu_1^{(j)}$, for $j \neq l + 1$, and the $(l + 1)$th entry is $-2 \sum_{j \neq l} m_e(x(v) \mu_1^{(j)}$. Finally, the first entry of $R_3$ is 0, and the rest, except the $(l + 1)$th entry, are $-m_e(x) \mu_0^{(j)} - m_e(x) \mu_0^{(j)}$, for $j \neq l + 1$, and the $(l + 1)$th entry is $m_e(x) \sum_{j \neq l} \mu_0^{(j)} + \sum_{j \neq l} m_e(x) \mu_0^{(j)}$. Consequently,

$$
E (\hat{m}(x) - m(x)) = \frac{1}{2} \mathbf{e}_1^T U_0^{-1} \left( h^2 R_0 + h(v - x) (R_1 - U_1 U_0^{-1} R_0) \right) + o(h(v - x)) + o(h^2) + O(\omega).
$$

To derive the asymptotic variance of $\hat{m}(x)$ we have

$$
Var(\hat{m}(x)) = \mathbf{e}_1^T (X^T W X)^{-1} (X^T W W X) (X^T W X)^{-1} \mathbf{e}_1,
$$

where $V = diag(f(x_1), \ldots, f(x_n))$, with $f(x_i) = (1/N \omega)m(x_i) - (1/N)m(x_i)^2$. We stress that $f(x_i)$ depends on $N$ and $\omega$, but we drop them from its notation for simplicity. Now use approximation
analogous to those used above we have

\[ \omega \sum_i (x_{ij} - v) K_h(x_{ij} - x)^2 f(x_{ij}) = f(x) R_1^{(j)} - \left( \frac{v - x}{h} \right) f(x) R_0^{(j)} - o \left( \frac{v - x}{h} \right) + O(\omega), \]

\[ \omega \sum_i (x_{ij} - v)^2 K_h(x_{ij} - x)^2 f(x_{ij}) \]

\[ = hf(x) R_2^{(j)} - 2(v - x)f(x) R_1^{(j)} + \left( \frac{v - x}{h} \right)^2 f(x) R_0^{(j)} + o(h) + o \left( \frac{(v - x)^2}{h} \right) + O(\omega), \]

\[ \omega \sum_i (x_{il} - x)^p K_h(x_{il} - x)^2 f(x_{ij}) = h^{p-1} f(x) R_p^{(j)} + o(h^{p-1}) + O(\omega), \text{ for } p = 0, 1, 2. \]

It follows that

\[ \omega X^T W V W X \]

\[ = \frac{1}{h} f(x) A \left[ M_0 + \left( \frac{v - x}{h} \right) M_1 + \left( \frac{v - x}{h} \right)^2 M_2 + o \left( \frac{v - x}{h} \right) \right] A, \]

where \( M_0 \) is symmetric, its first row is \( \sum_j R_0^{(j)}, R_1^{(j)}, \ldots, R_1^{(J)} \), and its diagonal entries are \( \sum_j R_0^{(j)}, R_2^{(1)}, \ldots, R_2^{(J)}. \) All the other entries of \( M_0 \) are zero. \( M_1 \) is symmetric, its first row is \( 0, -R_0^{(1)}, \ldots, -R_0^{(l-1)}, \sum_j R_0^{(j)}, -R_0^{(l+1)}, \ldots, -R_0^{(J)} \), its \( (l+1) \) th row is \( \sum_j R_0^{(j)}, R_1^{(1)}, \ldots, R_1^{(l-1)}, 0, R_1^{(l+1)}, \ldots, R_1^{(J)} \), and its diagonal is \( 0, -R_1^{(1)}, \ldots, -R_1^{(l-1)}, 0, -R_1^{(l+1)}, \ldots, -R_1^{(J)}. \) All other entries of \( M_1 \) are zero. Finally \( M_2 \) is also symmetric, its first row is the zero vector, its \( (l+1) \) th row is \( 0, -R_1^{(1)}, \ldots, -R_1^{(l-1)}, \sum_j R_0^{(j)}, -R_1^{(l+1)}, \ldots, -R_1^{(J)} \), and its diagonal is \( 0, R_0^{(1)}, \ldots, R_0^{(l-1)}, \sum_j R_0^{(j)}, R_0^{(l+1)}, \ldots, R_0^{(J)}. \) All other entries of \( M_2 \) are zero.

Combining the above expressions, we have

\[ \text{Var}(\hat{m}(x)) = C(N, h, \omega, x) \left[ U_0^{-1} M_0 U_0^{-1} + \left( \frac{v - x}{h} \right) U_0^{-1} (M_0 U_0^{-1} U_1 + M_1 - U_1 U_0^{-1} M_0) U_0^{-1} \right] \]

\[ + o \left( \frac{1}{Nh} \right) + o \left( \frac{\omega}{Nh} \right) + o \left( \frac{v - x}{Nh^2} \right) + o \left( \frac{\omega(v - x)}{Nh^2} \right). \tag{29} \]

\[ \square \]

**Supplementary Materials**

The supplementary materials include an R program containing code to perform the local linear regression method for density estimation on a network as described in this article. The program also contains all codes for simulating datasets used in the article.
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Figure 4: Equal-split discontinuous and continuous kernel estimator and diffusion estimator applied to the three cases. From left to right: case I, II and III.
Figure 5: The network is in red, and the true density functions over the network are the black dashed lines. **Left:** local piecewise linear estimation subject to joint equality of the regression functions at the vertex. **Right:** local piecewise linear estimation subject to that the first derivatives are jointly zero at the vertex.
Figure 6: Density estimation near vertices A, B, C and D.