Estimating animal densities and home range in regions with irregular boundaries and holes:

a lattice-based alternative to the kernel density estimator

Abstract Density estimates based on point processes are often restrained to regions with irregular boundaries or holes. We propose a density estimator, the lattice-based density estimator, which produces reasonable density estimates under these circumstances. The estimation process starts with overlaying the region with nodes, linking these together in a lattice and then computing the density of random walks of length k on the lattice. We use an approximation to the unbiased cross-validation criterion to find the optimal walk length k. The technique is illustrated using walleye (Sander vitreus) radiotelemetry relocations in Lake Monroe, Indiana. We also use simulation to compare the technique to the traditional kernel density estimate in the situation where there are no significant boundary effects.

Keywords: Diffusion, Point Process, Kernel Density Estimation, Intensity Functions, utilization distribution, home range
1 Introduction

Kernel density estimation is commonly used to estimate home ranges and utilization distributions of fish or wildlife (for instance, see Worton 1989). A significant problem with kernel estimators, however, is that they do not respect irregular boundaries or holes in regions. In estimating the home range of fish in a lake, for example, a kernel density estimator will place positive density along the shoreline or on islands within the lake.

A typical approach to remedying this problem is first to compute the estimator as if there were no boundaries, then to clip off inaccessible regions after the fact, and finally renormalize the density. But this solution is less than ideal. For instance, if there is a high density of fish in one lake and a second, closely located lake has no observed fish, the home range might end up including part of the apparently empty lake. One approach to this problem is the use of local convex hulls (Getz et al 2007; Getz and Wilmers 2004; Ryan et al. 2006).

In this paper we suggest an estimator of density based on an approximation to Brownian motion. Random walks, originating from each observation, are restrained to remain within the boundaries. This would be analogous to adding a quantity of dye to each location where a fish or animal was observed, then allowing the dye to diffuse outward. A density map based on the concentration of the dye at different times would result in a density estimator that is faithful to the boundaries of the region.

Our approach starts with a polygon that represents the region of interest. The polygon is filled with a grid of nodes, and a neighbor relationship is defined on the nodes to create a lattice in the sense of spatial lattice models (for instance, Cressie 1993, pp. 383 ff). The estimated density is derived from all length \( k \) random walks originating from the nodes where fish or other animals were located. The length, \( k \), of the random walk controls the smoothness of the resulting estimate. We propose a crossvalidation approach to select the optimal value of this smoothing parameter.

This density estimator we present has a number of desirable properties that make it preferable to existing methods. For instance, since the grid of nodes fills the polygonal region, the resulting density estimator will automatically give zero density outside the boundary. Where observations occur in a restricted part of the region, where nodes have fewer neighbors, the estimated density
will be higher, as expected. It is also straightforward to remove nodes within the region or links between nodes, accounting for holes such as islands in lakes and boundaries such as causeways, fences, etc. The lattice-based estimator uses a neighbor relationship between nodes filling a region, in contrast to the network-based kernel estimator of Downs and Horner (2007) which links observations into a network and uses kernel smoothing on the resulting network. The estimator is computationally fast, and we have written a set of functions in R (R core development team 2009) to implement it.

In this paper we first describe the method, the lattice-based density estimator, used to produce density maps. We then present a simple example that illustrates the computations in detail. Following this, we compare our method to a standard kernel density estimation method for a two dimensional point processes. Finally, we apply the method to estimate the density of walleye (*Sander vitreus*) in Lake Monroe, Indiana.

2 Theory/Calculations

2.1 Generating the density maps

A probability density is a function \( f(s) \) defined over a region \( A \) that allows the computation of the probability of locating an single object in a subregion \( B \) by integrating \( f \) over the subregion \( B \): 

\[
\int_B f(s) \, ds = P(\text{object in } B).
\]

In particular, areas where the density is high are areas where finding an object is likely. The minimal requirements of such a function are that 

\[
\int_A f(s) \, ds = 1,
\]

so that the probability of finding a specific object (i.e. one specific fish) somewhere in the region is 1, and that \( f(s) \geq 0 \), to avoid negative probabilities.

Given a point process of object locations, the true density can be estimated by means of a smoothing process, wherein areas in which large numbers of objects are found in a restricted are given high estimated densities. A density estimator \( \hat{f} \) should be a continuous function over our region and should be a bona fide density, that is its integral over the entire region should be one, and the estimated density should be non-negative everywhere.

Our approach is to discretize \( \hat{f} \) by choosing a set of \( N \) nodes (locations) in the region and defining a probability at each node such that the sum of the probabilities over all nodes is one.
relationship between the density estimate $\hat{f}$, which is defined everywhere over the region, and the probabilities at a node $s_i$ is that the node probabilities approximate the integral of $\hat{f}$ over a small region around $s_i$ with area $\text{area}(A)/N$. We will compute the probabilities at $s_1, \ldots, s_N$ from a random walk on the nodes, then obtain the estimated density from $\hat{f}(s_i)$ equal to the (discretized) probability at $s_i$ divided by $\text{area}(A)/N$. To find the discrete probability densities at $s_1, \ldots, s_N$ we need to define a lattice over these nodes.

A lattice consists of a set of $N$ nodes with NS and EW coordinates, and a neighbor relationship between pairs of nodes (Cressie 1993, pp. 383 ff). The neighbor relationship may be defined in many ways. Our implementation defines neighbors to be the closest nodes in the N, S, E, W, NE, NW, SE and SW directions, although it is possible to add links or remove them depending on the judgement of the researcher, for a particular data set. By definition the nodes are also their own neighbors.

Our estimator is the probability density of the length-$k$ random walk on the lattice. Let $X_k$ denote the position of the random walk at at step $k$. When $k = 0$ the estimated density is just the original set of observations, so that $P(X_0 = s_i) =$ the proportion of observed fish at location $s_i$. The random walk is just a finite state Markov chain, familiar to anyone who has worked with age-structured population models (Leslie 1945), with transition probabilities $P(X_{k+1} = s_i | X_k = s_j) \neq 0$ only if $s_i$ is a neighbor of $s_j$. Following standard Markov chain notation, the $N$ probability vector $p_k$ is

$$p_k = [P(X_k = s_1), \ldots, P(X_k = s_N)]$$

which shows the probability distribution after $k$ steps.

Define $T$ to be a $N \times N$ transition matrix in which the entry in the $i$th row and $j$th column is $P(X_{k+1} = s_j | X_k = s_i)$, the probability that a random walk at location $s_i$ moves to neighboring location $s_j$. From basic probability theory, $p_{k+1} = T p_k$, so that multiplying the probability density at time $k$ by $T$ produces the probability density after one step. By repeating this process, $p_k = T^k p_0$ gives the probability density of the random process after $k$ steps.
2.2 Properties of the transition matrix

For purposes of density estimation, especially mimicking the behavior of the usual kernel density estimator, it would be desirable that as $k$ gets very large, the density converges to the uniform (flat) density where $P(X_k = s_i) \approx 1/N$ at all locations when these locations are connected, since the ultimate smoothed estimator is constant everywhere in a connected region. Also, when there is no boundary and $k$ is moderately large, the density should be approximately the sum of normal kernels centered at each observation, so that in the no-boundary case the lattice-based estimator is comparable to the usual kernel density estimator.

In the no-boundary case, $X_k$ is a symmetric random walk centered on $X_0$, thus is the sum of $k$ independent and identically distributed random variables with finite variances, so that the central limit theorem makes the density approximate a bivariate normal density for moderate to large $k$.

A sufficient condition for the random process to ultimately become uniform is that $T$ be symmetric and all of the nodes connected in the sense that we can get from one node to any other by moving from node to neighboring node (Rosenblatt 1971). We add the further assumption that all movement probabilities are the same, so that the rate of movement of the random walk is the same everywhere. This is guaranteed by choosing the transition probabilities as follows: First, define $q_i$ to be the number of neighbors (other than itself) of the location $s_i$ (usually the maximum value for $q_i$ is 8 when a location is not near a boundary). Next, chose a parameter $M$ between zero and one. This parameter governs how often the random walk remains in the same location after one step. Then the transition probabilities are

$$P(X_{k+1} = s_i|X_k = s_i) = 1 - M \times (q_i/\max(q_i))$$ \hspace{1cm} (1)

and

$$P(X_{k+1} = s_j|X_k = s_i) = M \times \left(1/\max(q_i)\right) \text{ for } i \neq j$$ \hspace{1cm} (2)

In this paper we use $M = 0.5$. Generally the higher $M$ is, the more steps will be required to achieve the same degree of smoothing. The process as described above is a valid transition matrix and symmetric. To find the probabilities on $s_1, ..., s_N$, it remains only to choose the number of
steps \( k \). Then the estimated density is

\[
p_k = T^k p_0, \quad \hat{f}(s_i) = (N/\text{area}(A))p_{k,i}
\]  

(3)

2.3 Crossvalidation

As the number of steps \( k \) increases, the resulting density map becomes smoother. Selecting the optimal value of \( k \) is analogous to selecting the bandwidth in kernel density estimation. We suggest a crossvalidation approach. Here, for each observed fish or animal at location \( s_i \), we start with a probability density \( p_{0,-i} \) giving weight \( 1/(n-1) \) to all other observations and removing the \( i \)th observation. At step \( k \), define \( p_{k,i,-i} \) as the \( i \)th element in \( T^k p_{0,-i} \). What we are doing is removing the \( i \)th observation, then determining the density at location \( s_i \) after \( k \) steps. These are then combined into a measure of goodness-of-fit at \( k \) steps, the Unbiased Crossvalidation criterion UCV (Sain, Baggerly, Scott 1994):

\[
UCV_k = \int_{R^2} \hat{f}^2(x)dx - \frac{2}{n} \sum_{i=1}^{n} \hat{f}_{-i}(x_i)
\]

which we approximate by

\[
UCV_k = \frac{N}{\text{area}(A)} \sum_{j=1}^{N} p_j^2 - \frac{N}{\text{area}(A)} \frac{2}{n} \sum_{i=1}^{n} p_{k,i,-i}
\]  

(4)

where \( N \) is the number of nodes, \( n \) is the number of observation and \( \text{area}(A) \) is the area of the region. The optimal number of steps is that which minimizes \( UCV_k \).

2.4 Simple example

A very simple example should illustrate the mathematics of this technique. Figure (1) shows a polygon with a lattice consisting of six nodes and nine bidirectional links. Recall that \( q_i \) is the number of neighbors (not counting itself) of location \( s_i \). Here \( q_1 = 3, q_2 = 3, q_3 = 3, q_4 = 4, q_5 = 3, q_6 = 1 \). With \( M = 0.5 \), application of equation (1) yields the transition matrix \( T \):
Figure 1: Example lattice consisting of six nodes and nine bidirectional links inside a polygonal region.

\[ T = \begin{pmatrix}
0.625 & 0.125 & 0.125 & 0.125 & 0.000 & 0.000 \\
0.125 & 0.625 & 0.125 & 0.125 & 0.000 & 0.000 \\
0.125 & 0.125 & 0.500 & 0.125 & 0.125 & 0.000 \\
0.125 & 0.125 & 0.125 & 0.500 & 0.125 & 0.000 \\
0.000 & 0.000 & 0.125 & 0.125 & 0.625 & 0.125 \\
0.000 & 0.000 & 0.000 & 0.000 & 0.125 & 0.875
\end{pmatrix} \]

For instance this tells us that there is a 0.625 chance that a random walk at location 1 remains at location 1 after a single step, that there is a 0.125 chance that it moves from location 1 to location 2, and that there is no chance that it moves from location 1 to location 5 in a single step.

Note that the probability of movement from one node to a neighboring node is always 0.125 in this example and movement directly to a non-neighbor is impossible. Figure 1 shows the lattice with nodes labeled.

Suppose that one observation is recorded at location 1 and two observations are recorded at location 3. Then the initial probability density is \( p_0 = [0.3333, 0, 0.6667, 0, 0, 0] \). After a single step the density is \( p_1 = Tp_0 = [0.2916, 0.1250, 0.3750, 0.1250, 0.0833, 0.0000] \). One step isn’t sufficient, of course, to get non-zero probability at node 6, but the density is no longer concentrated only on nodes 1 and 3.

After two steps the density is more dispersed, with probability \( p_2 = T^2p_0 = [0.2604, 0.1770, 0.2656, 0.1718, 0.1145, 0.0104] \). After thirty steps the probability density has become close to uniform,
with probabilities $p_{30} = T^{30}p_0 = [0.1703, 0.1703, 0.1689, 0.1689, 0.1643, 0.1570]$. This diffusion process is illustrated in Figure 4.

2.5 Another example

The lattice-based density estimator performs well when there are convoluted boundaries. Consider the simulated point process displayed in Figure 3.

The point process was generated assuming a constant density for easting values less than 0.5 (see Figure 3). Clearly estimating density in this example with a standard approach that ignores the boundary information will not be able to prevent density from crossing the causeway and giving improper higher densities in areas just to the east of the causeway. We estimated the density with the lattice-based kernel estimator. A set of nodes spaced 0.01 units apart was juxtaposed over the polygon. Crossvalidation yielded a minimum UCV at $k = 176$ steps. The large number of steps is reasonable, since we would expect the map to be quite smoothed since the true density is uniform over much of the polygon. The resulting density map is shown in Figure 4.

Note that the density estimate is positive in the eastern side of the polygon where there is an opening in the causeway, but not in other areas east of the causeway.
Figure 3: A complicated polygon, with a point process restricted west of a causeway.

Figure 4: Lattice-based density estimate based on $k = 176$ steps.
3 Simulation

We performed a small simulation study to compare the performance of our estimator to that of the usual bivariate kernel density estimator. Since the typical kernel estimator does not account for irregular boundaries or holes, we computed both estimators over a square region. Thus this simulation only considers the situation where the boundary does not matter. However the results can be used to infer the performance of our estimator over a more complex region.

In each simulation we generated $n = 100$ observations, $(X_j, Y_j)$ for $j = 1, \ldots, 100$, from the multivariate normal distribution with mean and covariance

$$\mu = \begin{bmatrix} 5 \\ 5 \end{bmatrix} \quad \text{and} \quad \Sigma = \begin{bmatrix} 1.5 & 0.8 \\ 0.8 & 1.5 \end{bmatrix}.$$  

Data were generated using the R package \texttt{mnormt} (Genz and Azzalini 2009).

For each simulated data set we computed the lattice-based density estimator in Equation (3) with $h$ chosen by minimizing the UCV criterion in (4), and the bivariate kernel density estimator (Venables and Ripley 2002),

$$\hat{f}(x, y) = \frac{1}{nh_1 h_2} \sum_{j=1}^{n} \phi \left( \frac{x - X_j}{h_1} \right) \phi \left( \frac{y - Y_j}{h_2} \right),$$

where $\phi$ is the Gaussian kernel and $h_1$ and $h_2$ are bandwidth parameters. Bandwidths for the kernel estimator were also chosen by Unbiased Crossvalidation (Venables and Ripley 2002). This estimator and its bandwidth were computed with the R functions \texttt{kde2d} and \texttt{ucv} in the package \texttt{MASS} (Venables and Ripley 2002). Both estimators were computed on a $16 \times 16$ grid from -10 to 10 in both $x$ and $y$ directions.

Estimators were compared based on their average Integrated Squared Error (ISE), defined for an estimator $\hat{f}(x, y)$ as

$$ISE\{\hat{f}(x, y)\} = \int \int \left\{ f(x, y) - \hat{f}(x, y) \right\}^2 dx dy.$$

Results are based on 100 simulated data sets.

The normal target density, along with one realization of the bivariate kernel and lattice-based density estimators, are displayed in Figure 5. In terms of average ISE, the lattice-based density estimator actually performed significantly better than the two-dimensional kernel density estimator.
Figure 5: The true density, a kernel density estimate and a lattice-based density estimate

Figure 6: Boxplots of average ISE for the lattice-based and kernel estimators.

when compared using a paired t-test (p-value = 0.00169). There was also less variation in ISE for the lattice-based density estimator than the kernel estimator. Boxplots of the ISEs are displayed in Figure 6.

4 Application

We illustrate our method using data supplied by Sandra Clark-Kolaks based on radiotelemetry relocations of walleye (Sander vitreus) in Lake Monroe, Indiana (Clark-Kolaks 2009). Data from three widely-separated days, 16 October 2008 (15 relocations), 17 March 2009 (19 relocations) and 9 April 2009 (16 relocations), were pooled for a total of 50 relocations. These relocations are plotted within the polygonal representation of Lake Monroe in Figure 7. It is clear that the standard
kernel approaches will be problematic in estimating walleye home range in the lake. Many of the relocations are along the boundary of the lake, there is a narrow causeway almost bisecting the lake and some of the fish have been located in narrow bays.

We used the lattice-based density estimator to estimate walleye home range. Nodes were spaced 200 m apart within the polygon, to cover the entire lake. The lattice was constructed in two steps. First, all pairs of nodes between 100 m and 300 m were declared neighbors. Often this is sufficient, but in this case the convoluted nature of the lake shore required some editing of the neighbor structure. Three nodes had no neighbors at all and some pairs of nodes that were separated by land were neighbors. An editing function in R, `edit.lattice`, was used to hand-edit the neighbor structure.

Figure 7 shows a close look at the causeway and illustrates the neighbor relationship, where neighbors are connected by line segments.
Crossvalidation on the data resulted in a minimum UCV at 7 steps. The approximate UCV at different values of $k$ is displayed in Figure 9. The lattice-based density estimator was computed with this number of steps, and a contour map of the resulting estimate is shown in Figure 10. Note that the lattice-based density estimator shows higher densities in narrow bays in which fish were observed.

A common approach to defining a home range is to find the smallest area that contains a given proportion $P$ of the density, i.e. a subregion $B$ of minimal area such that $\int_B \hat{f}(s)\,ds = P$. We find such a region simply by finding the smallest number of nodes that have a probability totalling at least $P$. Figure 11 shows the minimal area where the nodes account for at least $P = 0.75$.

5 Discussion

The presence of boundaries and holes in regions has been problem for the typical implementation of kernel density estimators for home range or utilization distribution studies. The lattice-based density estimator adjusts densities for boundaries and holes, and is as implemented in R fairly straightforward to use. In the absence of boundaries and with elliptical true densities the lattice-
Figure 9: Crossvalidation criterion for different numbers of steps $k$.

Figure 10: Contour map of the lattice-based estimator of walleye home range in Lake Monroe.
based estimator works as well as the typical kernel density estimator so there is no reason not to use the lattice-based approach. Because bandwidth can be obtained through crossvalidation, the only decision required of the researcher is deciding on the spacing of the nodes, which realistically should be as small as possible, limited by the computation time and memory required. For the Lake Monroe data, on a fairly antiquated laptop computer (Dell Inspiron 9300, running Windows XP at 1.6 GHz with 2 GB of RAM) the generation of the nodes and lattice required 4 seconds while the crossvalidation required only 8 additional seconds. However, reducing the node spacing down from 200 meters to 50 meters made the functions run very slowly as too much memory was required. All of the R functions are available as an R package from the authors.

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