Comparison of least-squares cross-validation bandwidth options for kernel home-range estimation

Robert A. Gitzen and Joshua J. Millspaugh

Abstract In radiotracking studies, kernel estimation commonly is used to calculate an animal's utilization distribution from location data. A major limitation of kernel-based methods is their high sensitivity to bandwidth values. Least-squares cross-validation (LSCV) is the recommended default bandwidth selection method in ecological literature and is widely available in home-range software. However, various forms of the LSCV method may perform differently in terms of bias and precision. We used simulations to compare the performance of several LSCV forms, including the commonly used scaling approach, as well as sphering, bivariate score function, and univariate alternatives. We combined 2, 4, or 16 bivariate normal distributions and generated sample sizes of 50 or 150 points from each mixture distribution. We calculated absolute bias in home-range size estimates at contours of 99, 95, 75, 50, and 25%. Using the Volume of Intersection (VI) Index, we examined surface fit between each estimated and true distribution. All LSCV forms generally were better than the reference bandwidth. No LSCV option was uniformly best, but the scaling and sphering approaches were slightly better across all contours. Univariate LSCV was similar to other options at outer contours and in surface fit but performed worse at inner contours and was most inconsistent. Using the global versus largest local minimum was unimportant in our comparisons. Although differences among LSCV options were small, these differences could add to variability of kernel estimates across studies. Further evaluation of "second generation" methods (e.g., plug-in approaches) is warranted.

Key words bandwidth, fixed kernel, home range, least-squares cross-validation, LSCV, Monte Carlo simulations, smoothing parameter, space use, utilization distribution, volume of intersection

Since its first application to home-range estimation by Worton (1987, 1989), kernel density estimation has become a standard technique for estimating home-range size and other features of an animal's utilization distribution (UD; Van Winkle 1975; Fig. 1). Perhaps the biggest drawback of kernel estimators is their sensitivity to the choice of bandwidth values (smoothing parameters; Silverman 1986, Worton 1995, Seaman et al. 1999). Different bandwidth values applied to the same data set may dramatically affect the shape of the estimated UD (Kernohan et al. 2001) and the estimated home-range size (Seaman and Powell 1996).

A simple bandwidth selection method is the "normal" or "reference" smoothing parameter (h_{ref}), which estimates the bandwidth that would minimize error if the data came from a bivariate normal distribution (Silverman 1986). This method often oversmooths for more realistic multi-modal data (Wand and Jones 1995). Currently, LSCV is recommended as the default bandwidth selection method in ecological studies (Worton 1995, Seaman and Powell 1996, Seaman et al. 1999) and in home-range estimation programs that incorporate kernel estimation (e.g., Hooge and Eichenlaub 1997, Seaman et al. 1998).

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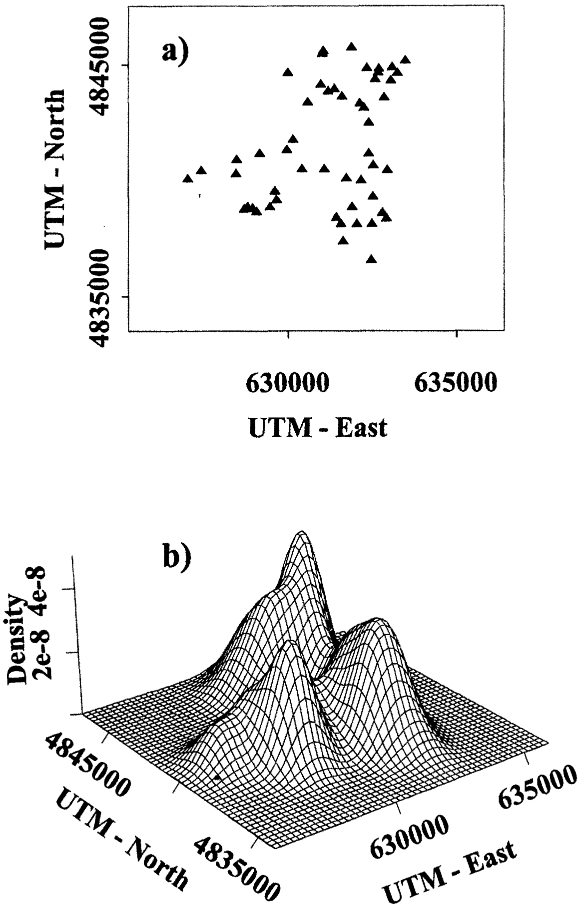

Figure 1. (a) Fifty-two radiotracking locations of a yearling cow elk (*Cervus elaphus*) in fall 1993 at Custer State Park, South Dakota, USA (see Millspaugh et al. 2000 for methods). (b) Estimated utilization distribution calculated from these points with fixed-kernel method and scaling version of least-squares cross-validation. Selected bandwidths = (534, 868). Kernel plotting routine from Bowman and Azzalini (1997).

As with other options (Lawson and Rodgers 1997), variation among LSCV implementations could contribute to inconsistency of home-range estimates from different software packages. The LSCV bandwidth is calculated by minimizing a score function over a suitable range of values (Silverman 1986). Previous home-range studies (Seaman and Powell 1996, Seaman et al. 1999) used the LSCV score function for bivariate data presented by Silverman (1986). With this scaling approach (Wand and Jones 1993, Seaman and Powell 1996), the data are standardized to have equal variances for both coordinates and a LSCV score function based on a single bandwidth value is minimized. This value is multiplied by the standard deviations of the unscaled data for each coordinate to produce the bandwidth vector $\mathbf{h}=(h_x, h_y)$.

A similar variation is the "sphering" approach (Wand and Jones 1993). Data are sphered to be standard bivariate normal (variances=1 and covariances=0), the LSCV score function based on a single value of h is minimized, and then the minimum is multiplied by the original covariance matrix to produce a bandwidth matrix with h_x, h_y, and h_{xy}. Use of 3 bandwidth values allows smoothing to be oriented away from the x- and y-coordinates, but the sphering approach may be an overly simplistic way to estimate the full bandwidth matrix (Wand and Jones 1993). An alternative LSCV bivariate score function includes (h_x, h_y) directly, so that minimization of a score function of 2 variables is necessary (Sain et al. 1994).

Finally, for bivariate data, separate univariate LSCV bandwidths can be calculated for the x- and y-data vectors and then combined to form (h_x, h_y). Such an approach may be desirable if the analyst wishes to estimate home-range size in a general-purpose statistical program that incorporates only the univariate LSCV calculations. For any of the LSCV methods, the score function may have multiple local minima, and the recommended approach is to use the largest local minimum instead of the global minimum (Park and Marron 1990).

Wand and Jones (1993) analytically calculated optimal (error-minimizing) bandwidths for several mixture distributions and bandwidth parameterizations. They concluded that scaling and sphering approaches can perform poorly and did not recommend them except for unimodal normal distributions. Evaluation of these approaches is needed to determine whether Wand and Jones' (1993) conclusion should affect how home-range programs implement the LSCV method.

We questioned whether differences among these LSCV options were important to kernel home-range estimation and whether any options outperform the scaling approach used in previous studies. As current home-range packages do not specify whether LSCV implementations seek a global or largest local minimum, we examined the importance of this choice. Using simulated data, we evaluated the degree to which LSCV performance varies among these options for the fixed-kernel method.

Methods

Simulations

Similar to previous studies (Seaman and Powell

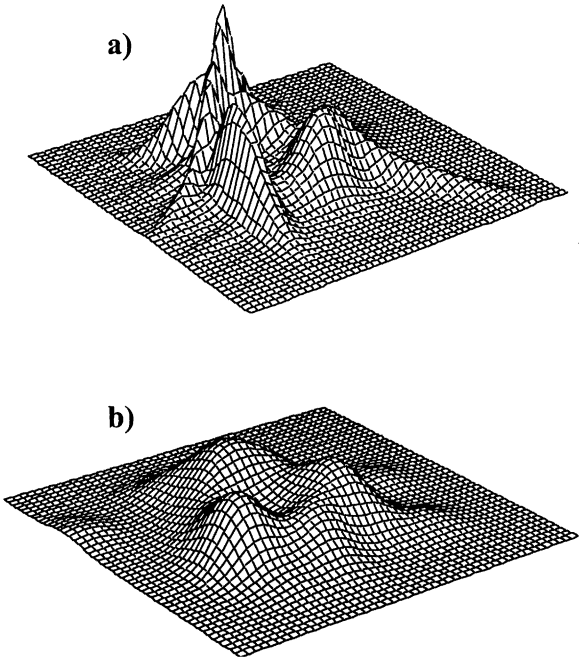

Figure 2. (a) Mixture distribution of 16 random bivariate normal distributions. (b) Distribution estimated with fixed-kernel method based on 50 random points from the mixture distribution and bandwidth selected by the scaling version of least-squares cross-validation. Height above *x*- and *y*-plane is the true or estimated density *f*(*x*). Axes have the same scale on both figures; the estimated distribution underestimates the sharp peaks of the true distribution. Estimated and true distributions had a Volume of Intersection of 0.76. Bias in "home-range size" estimates: 0.2% (99% contour), 7.1% (95% contour), 15.9% (75% contour), 35.3% (50% contour), and 52.5% (25% contour).

1996, Seaman et al. 1999), we based our simulations on bivariate normal mixture distributions (Fig. 2). These mixture distributions are simplified models of animal space use, but were appropriate given our focus on relative performance among bandwidth options. This approach allowed a clear comparison of bandwidth performance across a wide range of distribution patterns.

We compared LSCV options across 2 factors: the number of bivariate normals in each mixture distribution (2, 4, or 16) and the sample size ($n = 50$ or $n = 150$). For each combination of sample size and number of normals, we performed 500 replications. For each replication, we randomly selected a mixture distribution. The mixture distribution followed Seaman et al. (1999), with the variance for each coordinate in each normal in the mixture randomly chosen from the uniform distribution between 1 and 36. The x- and y-mean parameters for each bivariate normal in the mixture were chosen separately from the uniform distribution between 0 and 20. The correlation parameter was chosen from the uniform distribution in the interval (-1, 1). Mixing proportions for the normals in each mixture were chosen randomly and constrained to sum to 1. We performed simulations in MATLAB 5.3 (The Mathworks Inc., Natick, Mass.). We created MATLAB functions to calculate bandwidth values and perform other simulation procedures. We used a function from Beardah and Baxter (1995) to calculate kernel density estimates. For the sphering approach, we used the function from Beardah and Baxter (1995) as a guide, and wrote a routine to calculate density estimates when 3 bandwidth values are used.

Bandwidth calculations

We focused on the fixed-kernel method, where the same bandwidth is used for smoothing all observations in a data set. Although the relative performance of fixed- versus adaptive-kernel methods depends on the bandwidth method and the question of interest (Kernohan et al. 2001), fixed kernels generally are superior for estimating the outer contours of the home range and for estimating the UD surface (Seaman et al. 1999). All calculations used a normal kernel (Silverman 1986).

For each replication, we calculated bandwidth values for the random sample of points. For comparison with the LSCV options, we calculated the reference bandwidth as in Seaman and Powell (1996), with $n^{-1/6}$ multiplied by the standard deviation for each coordinate vector (i.e., $\mathbf{h}_{ref} = [n^{-1/6} \times \sigma_x, n^{-1/6} \times \sigma_y]$, where n = sample size). (Note that this differs slightly from Silverman [1986] and Worton [1995], who used a single value of h for both coordinates.) We evaluated several variations of the LSCV method, including the standard scaling approach used by Seaman and Powell (1996), the sphering approach, the bivariate score function approach incorporating 2 bandwidths directly (Sain et al. 1994), and the "separate univariate approach" in which bandwidths are calculated using the score function for univariate data. For the scaling, sphering, and univariate approaches, we searched for both the global and largest local minimum in the score function. For the bivariate score function approach, we searched only for a local minimum in the neighborhood of h_{ref}. We, therefore, calculated 7 LSCV bandwidths.

For all LSCV options, we searched for the score function minimum within the interval ($0.1 \times h_{ref}, 2 \times h_{ref}$). For the scaling, sphering, and univariate approaches, we searched for the global minimum in the appropriate score function by direct search over 300 possible bandwidth values equally spaced in the search interval. This brute-force search strategy, although less efficient than other optimization methods, was suitable for automatic application to a large number of simulated data sets and facilitated the search for a local minimum. Additional comparisons indicated that this brute-force method matched the performance of numerical optimization strategies. For each score value, we calculated the difference $\text{score}_i - \text{score}_{i-1}$, where $i=2$ to 300, corresponding to each bandwidth in the search interval except the lowest value. This difference is negative where the score function is decreasing to a minimum. The largest bandwidth value with this negative slope was taken as the largest local minimum unless the bandwidth was on the search interval boundary. We minimized the bivariate score function using the MATLAB Optimization Toolbox 2.0 function "fmincon" for constrained nonlinear minimization. For each LSCV approach, when the score function minimum was at the upper or lower bound of the search interval, we classified this as failure of that LSCV option but set the bandwidth equal to h_{ref}. Few identical points or very tight clusters existed within each of our simulated point sets, so LSCV rarely failed.

Use of a univariate bandwidth method requires modification of the selected bandwidth values when the data are multidimensional (Ćwik and Koronacki 1997). For bivariate data, Ćwik and Koronacki (1997) raised each univariately selected coordinate bandwidth to the 5/6 power. We used this rule of thumb for the univariate LSCV method. Our additional data (R. A. Gitzen and J. J. Millspaugh, unpublished data) indicated that raising each coordinate bandwidth selected by the univariate LSCV approach to the 5/6 power produced estimated UDs with higher VI scores and lower absolute percent bias in home-range estimates at outer contours compared to the untransformed bandwidths.

Bandwidth comparisons

We calculated the true mixture density and the estimated fixed-kernel density for each bandwidth value at a grid of 52,900 points. The mixture density $f_{x,y}$ was calculated as

$$f_{x,y} = \sum_{i=1}^{n} p_i \phi_i(x,y),$$

where n is number of normals in the mixture (2, 4, or 16), p_i is the mixing proportion for each normal distribution, and $\phi_i(x,y)$ is a bivariate normal density function (Wand and Jones 1993). We calculated the volume contours corresponding to the minimum areas containing 99, 95, 75, 50 and 25% of the true distribution volume and estimated the corresponding home-range areas for the UD estimated with each bandwidth method. For each replicate we calculated percent absolute bias (PAB) between the true (T) and estimated (E) home-range sizes for each contour level, where $\text{PAB} = 100 \times |E-T|/T$. We used the VI Index (Seidel 1992, Millspaugh et al. 2000) to measure the overall fit of estimated and true UDs. We calculated the VI Index between the true UD and the estimated UD for each bandwidth. The VI Index measures overlap between these utilization distributions by

$$\text{VI} = \iint \min\left(f_1(x,y), \hat{f}_2(x,y)\right) dxdy,$$

where f_1 is the true mixture distribution and $\hat{f}_2$ is the estimated distribution. The VI statistic is bounded between 0 and 1 because each utilization distribution has a volume of 1. In our study the VI Index measures the fit of the estimated to the true distribution.

For each combination of design factors, we calculated the mean percent absolute bias in home-range size estimates at each contour and the mean VI score. We ranked the 7 LSCV options for each simulation by VI score and calculated the frequency that each LSCV bandwidth produced the highest and lowest scores.

Results

Except for a sample size of 50 from mixtures of 16 normals, all LSCV options produced more accurate estimates of home-range area than h_{ref} at all contours (Tables 1-5). This difference was accentuated at inner contours, where the comparative performance of h_{ref} was worst (Table 5). The reference bandwidth also produced VI scores that were lower and more variable among simulations than the LSCV options, although the differences in mean scores were relatively low (Table 6). Overall, h_{ref} produced VI scores lower than all 7 LSCV options in 44% (1,329 of 3,000) of simulations.

In average performance the largest differences among LSCV options were between univariate

Table 1. Mean (SE) absolute percent bias in home range estimates at the 99% contour for the reference bandwidth and 7 least-squares cross-validation bandwidth selection options. Samples of n = 50 or n = 150 points were drawn from simulated mixture distributions composed of 2, 4, or 16 bivariate normals. Based on 500 distributions for each combination of sample size and number of normals.

	n = 50			n = 150		
	2 normals	4 normals	16 normals	2 normals	4 normals	16 normals
Reference	46.5 (2.4)	40.0 (1.4)	24.3 (0.7)	42.1 (2.0)	34.1 (1.2)	20.3 (0.5)
Bivariate	22.5 (0.8)	22.9 (0.8)	25.0 (0.9)	14.1 (0.5)	16.0 (0.6)	12.3 (0.4)
Scale GM[a]	23.0 (0.8)	23.3 (0.8)	25.5 (0.9)	14.2 (0.5)	16.3 (0.6)	12.0 (0.4)
Scale LLM[b]	23.0 (0.8)	23.3 (0.8)	25.5 (0.9)	14.2 (0.5)	16.3 (0.6)	12.0 (0.4)
Sphere GM	23.4 (0.8)	23.3 (0.8)	25.7 (0.9)	13.9 (0.5)	16.2 (0.6)	12.2 (0.4)
Sphere LLM	23.4 (0.8)	23.3 (0.8)	25.6 (0.9)	13.9 (0.5)	16.1 (0.6)	12.1 (0.4)
Univariate GM	26.1 (1.1)	22.0 (0.8)	19.0 (0.6)	17. 3 (0.9)	14.9 (0.6)	12.8 (0.5)
Univariate LLM	26.1 (1.2)	21.1 (0.7)	17.6 (0.6)	17.2 (0.9)	14.5 (0.6)	11.7 (0. 4)

[a] GM = global minimum.
[b] LLM = largest local minimum.

Table 2. Mean (SE) absolute percent bias in home range estimates at the 95% contour for the reference bandwidth and 7 least-squares cross-validation bandwidth selection options. Samples of n = 50 or n = 150 points were drawn from simulated mixture distributions composed of 2, 4, or 16 bivariate normals. Based on 500 distributions for each combination of sample size and number of normals.

	n = 50			n = 150		
	2 normals	4 normals	16 normals	2 normals	4 normals	16 normals
Reference	57.5 (2.7)	49.7 (1.6)	32.6 (0.8)	51.5 (2.2)	43.0 (1.4)	27.2 (0.5)
Bivariate	25.2 (0.8)	25.0 (0.8)	29.0 (1.0)	15.4 (0.5)	15.5 (0.5)	13.9 (0.5)
Scale GM[a]	25.5 (0.9)	24.9 (0.9)	29.7 (1.0)	15.5 (0.5)	15.1 (0.5)	13.9 (0.5)
Scale LLM[b]	25.6 (0.9)	24.9 (0.9)	29.7 (1.0)	15.5 (0.5)	15.1 (0.5)	13.9 (0.5)
Sphere GM	25.6 (0.9)	24.9 (0.8)	29.6 (1.0)	15.3 (0.5)	15.0 (0.5)	13.8 (0.5)
Sphere LLM	25.6 (0.9)	24.9 (0.8)	29.6 (1.0)	15.3 (0.5)	14.9 (0.5)	13.8 (0.5)
Univariate GM	29.0 (1.3)	23.7 (0.9)	19.9 (0.7)	19.3 (1.0)	15.6 (0.7)	11.9 (0.4)
Univariate LLM	29.9 (1.5)	23.7 (0.9)	19.5 (0.7)	20.1 (1.1)	15.7 (0.7)	11.6 (0.4)

[a] GM = global minimum.
[b] LLM = largest local minimum.

Table 3. Mean (SE) absolute percent bias in home range estimates at the 75% contour for the reference bandwidth and 7 least-squares cross-validation bandwidth selection options. Samples of n = 50 or n = 150 points were drawn from simulated mixture distributions composed of 2, 4, or 16 bivariate normals. Based on 500 distributions for each combination of sample size and number of normals.

	n = 50			n = 150		
	2 normals	4 normals	16 normals	2 normals	4 normals	16 normals
Reference	76.3 (4.3)	66.3 (2.2)	39.4 (1.0)	65.5 (2.9)	58.1 (2.1)	31.4 (0.6)
Bivariate	31.5 (1.0)	29.9 (1.0)	33.3 (1.1)	19.2 (0.5)	17.4 (0.5)	16.8 (0.5)
Scale GM[a]	32.3 (1.0)	30.4 (1.0)	34.2 (1.1)	19.2 (0.5)	17.1 (0.5)	17.0 (0.5)
Scale LLM[b]	32.5 (1.0)	30.4 (1.0)	34.2 (1.1)	19.2 (0.5)	17.1 (0.5)	17.0 (0.5)
Sphere GM	31.7 (1.0)	30.4 (1.0)	34.1 (1.1)	19.0 (0.5)	16.9 (0.5)	16.9 (0.5)
Sphere LLM	31.8 (1.0)	30.4 (1.0)	34.1 (1.1)	19.0 (0.5)	16.9 (0.5)	17.0 (0.5)
Univariate GM	38.3 (2.0)	30.7 (1.2)	24.1 (0.8)	25.9 (1.5)	21.7 (1.0)	14.0 (0.5)
Univariate LLM	40.6 (2.5)	31.7 (1.2)	24.6 (0.8)	27.2 (1.5)	22.2 (1.1)	14.4 (0.5)

[a] GM = global minimum.
[b] LLM = largest local minimum.

Table 4. Mean (SE) absolute percent bias in home range estimates at the 50% contour for the reference bandwidth and 7 least-squares cross-validation bandwidth selection options. Samples of n = 50 or n = 150 points were drawn from simulated mixture distributions composed of 2, 4, or 16 bivariate normals. Based on 500 distributions for each combination of sample size and number of normals.

	n = 50			n = 150		
	2 normals	4 normals	16 normals	2 normals	4 normals	16 normals
Reference	94.4 (5.5)	91.5 (4.0)	47.5 (1.2)	80.2 (3.9)	80.3 (3.3)	38.9 (0.9)
Bivariate	35.7 (1.3)	37.3 (1.4)	38.1 (1.3)	22.2 (0.7)	21.7 (0.7)	20.8 (0.6)
Scale GM[a]	38.3 (1.4)	39.3 (1.5)	40.1 (1.3)	22.8 (0.7)	22.3 (0.7)	21.7 (0.6)
Scale LLM[b]	38.4 (1.4)	39.3 (1.5)	40.1 (1.3)	22.8 (0.7)	22.3 (0.7)	21.8 (0.6)
Sphere GM	37.7 (1.3)	39.3 (1.5)	39.9 (1.3)	22.4 (0.7)	22.2 (0.7)	21.5 (0.6)
Sphere LLM	37.8 (1.3)	39.3 (1.5)	39.9 (1.3)	22.4 (0.7)	22.2 (0.7)	21.6 (0.6)
Univariate GM	46.6 (2.9)	41.8 (2.0)	29.0 (1.0)	32.7 (2.3)	31.0 (1.7)	18.5 (0.6)
Univariate LLM	49.9 (3.3)	43.5 (2.0)	29.8 (1.0)	34.2 (2.4)	31.8 (1.7)	19.1 (0.6)

[a] GM = global minimum.
[b] LLM = largest local minimum.

Table 5. Mean (SE) absolute percent bias in home range estimates at the 25% contour for the reference bandwidth and 7 least-squares cross-validation bandwidth selection options. Samples of n = 50 or n = 150 points were drawn from simulated mixture distributions composed of 2, 4, or 16 bivariate normals. Based on 500 distributions for each combination of sample size and number of normals.

	n = 50			n = 150		
	2 normals	4 normals	16 normals	2 normals	4 normals	16 normals
Reference	112.8 (7.0)	144.4 (9.5)	67.2 (1.9)	94.7 (5.4)	127.5 (10.2)	57.3 (1.5)
Bivariate	40.3 (1.8)	55.0 (3.0)	51.4 (1.8)	24.4 (0.9)	31.7 (1.7)	30.5 (1.0)
Scale GM[a]	46.1 (2.9)	59.3 (3.1)	55.3 (1.9)	25.6 (0.9)	33.7 (1.7)	32.7 (1.0)
Scale LLM[b]	46.2 (2.9)	59.3 (3.1)	55.3 (1.9)	25.6 (0.9)	33.7 (1.7)	32.7 (1.0)
Sphere GM	44.2 (1.9)	59.5 (3.2)	55.1 (1.9)	25.4 (0.9)	33.9 (1.8)	32.4 (1.0)
Sphere LLM	44.2 (1.9)	59.5 (3.2)	55.1 (1.9)	25.4 (0.9)	33.9 (1.8)	32.6 (1.0)
Univariate GM	55.2 (4.1)	67.5 (5.1)	39.8 (1.6)	38.9 (3.4)	51.9 (4.7)	28.5 (1.0)
Univariate LLM	59.4 (4.5)	71.1 (5.5)	41.5 (1.6)	40.7 (3.5)	53.2 (4.7)	29.7 (1.0)

[a] GM = global minimum.
[b] LLM = largest local minimum.

Table 6. Mean (SE) Volume of Intersection scores for the reference bandwidth and 7 least-squares cross-validation bandwidth selection options for sample sizes of n = 50 or n = 150 and distributions formed by combining 2, 4, or 16 random bivariate normal distributions. Based on 500 distributions for each combination of sample size and number of normals.

	n = 50			n = 150		
	2 normals	4 normals	16 normals	2 normals	4 normals	16 normals
Reference	0.73 (0.005)	0.71 (0.004)	0.76 (0.002)	0.77 (0.005)	0.76 (0.004)	0.80 (0.002)
Bivariate	0.75 (0.003)	0.73 (0.003)	0.74 (0.002)	0.82 (0.002)	0.80 (0.003)	0.80 (0.002)
Scale GM[a]	0.76 (0.003)	0.73 (0.003)	0.75 (0.002)	0.82 (0.002)	0.80 (0.003)	0.81 (0.002)
Scale LLM[b]	0.76 (0.003)	0.73 (0.003)	0.75 (0.002)	0.82 (0.002)	0.80 (0.003)	0.81 (0.002)
Sphere GM	0.76 (0.003)	0.73 (0.003)	0.75 (0.002)	0.83 (0.002)	0.80 (0.003)	0.81 (0.002)
Sphere LLM	0.76 (0.003)	0.73 (0.003)	0.75 (0.002)	0.83 (0.002)	0.80 (0.003)	0.81 (0.002)
Univariate GM	0.74 (0.003)	0.72 (0.003)	0.74 (0.003)	0.81 (0.003)	0.79 (0.003)	0.80 (0.002)
Univariate LLM	0.75 (0.003)	0.73 (0.003)	0.75 (0.002)	0.81 (0.003)	0.79 (0.003)	0.80 (0.002)

[a] GM = global minimum.
[b] LLM = largest local minimum.

Table 7. Percent of simulations in which each of 7 least-squares cross-validation options[a] ranked best or worst in Volume of Intersection scores for sample sizes of n = 50 or n = 150 points and distributions formed by combining 2, 4, or 16 random bivariate normal distributions. Based on 500 distributions for each combination of sample size and number of normals. Sum of percentages for each sample size/number of normals exceeds 100 due to ties in ranks.

	% of distributions ranked best						% of distributions ranked worst					
	n = 50			n = 150			n = 50			n = 150		
Normals	2	4	16	2	4	16	2	4	16	2	4	16
Bivariate	13	17	12	26	28	17	25	28	32	16	18	30
Scale GM[b]	14	16	26	16	18	24	13	12	9	9	13	6
Scale LLM[c]	14	16	26	16	18	24	13	12	9	9	13	6
Sphere GM	41	27	20	38	28	26	19	25	20	24	24	20
Sphere LLM	41	27	20	38	28	26	19	25	20	24	24	20
Univariate GM	28	34	37	18	25	28	41	35	39	50	44	45
Univariate LLM	31	39	41	20	26	32	36	28	32	46	42	38

[a] To focus comparisons on LSCV options, the reference bandwidth was not ranked.
[b] GM = global minimum.
[c] LLM = largest local minimum.

LSCV and the other options (scaling, sphering, and bivariate) in absolute home-range bias. Sample size affected bias and surface fit much more than the choice of LSCV option. Mean VI scores varied among LSCV options by only 0.01-0.02 at a fixed sample size and distribution complexity (Table 6). For each LSCV option, mean VI scores increased by 0.05-0.07 when the sample size increased from 50 to 150. This pattern also was observed for absolute bias in home-range size at all contours. However, choice of LSCV versus h_{ref} usually had a greater impact on bias than choosing a sample size of 150 versus 50 for a given LSCV option.

Mean VI scores changed little as distribution complexity (number of normals) increased. For most LSCV options, home-range size bias varied more across the number of normals, but effects were minor compared to sample size differences. However, absolute bias of the univariate LSCV decreased as distribution complexity increased. For mixtures of 2 or 4 normals, the univariate LSCV performed worse than other LSCV options, with high bias at inner contours. For mixtures of 16 normals, the univariate LSCV had lower absolute bias than other LSCV options, with the largest differences at inner contours.

The univariate LSCV showed a similarly inconsistent pattern in ranked VI performance (Table 7). This method often had either the highest or the lowest VI scores. Even with complex distributions, the univariate LSCV had the lowest VI score in 32-45% of simulations. The scaling LSCV approach showed the opposite pattern, with low percentages of highest or lowest VI scores. Differences were low among VI scores and among home-range bias contours at outer contours for the scaling, sphering, and bivariate LSCV options (Tables 1-2, Tables 6-7). At contours of 50 and 25%, differences between the bivariate LSCV and the scaling/sphering LSCV average absolute biases were greater, with the bivariate LSCV having lower bias (Tables 4-5). However, these differences were still small compared to differences between each of these options and h_{ref} (Tables 3-5).

For scaling and sphering LSCV options, the global and largest local minima were nearly always identical (Tables 1-7), differing in only 3 (scaling) and 7 (sphering) distributions out of 3,000. The global and largest local minima were different more frequently for the univariate LSCV (258 of 3,000 distributions), although the average estimates differed only slightly. For average absolute bias, the univariate global minimum performed slightly better than the largest local minimum (Tables 1-5), but the opposite was true for VI scores (Table 7).

Discussion

Our study was motivated by concern that current home-range software may be using inferior forms of the LSCV method and that differences in LSCV options may complicate home-range comparisons. Based on Wand and Jones (1993), we expected that the bivariate score function for LSCV would outperform the scaling approach used previously, as well as the sphering approach. Instead, differences were slight except at inner contours, where the bivariate LSCV was somewhat better. No LSCV option was uniformly best, but the scaling approach was as good as any at outer contours and in VI scores. Moreover, using the global versus largest local minimum was largely unimportant in our comparisons. For the distributions we simulated, the global minimum in each score function generally was the same as the largest local minimum.

However, we did not create point patterns with many identical or very tightly clumped locations. Further evaluation of such point patterns is needed before concluding that this issue can be ignored.

For general bandwidth parameterizations, Wand and Jones (1993) concluded that direct estimation of 2 (as in the bivariate score function approach) or 3 bandwidth values is superior to scaling or sphering approaches. However, Wand and Jones (1993) analytically calculated optimal bandwidths for selected mixture distributions and purposefully did not consider bandwidth selection uncertainty. In our study, this uncertainty may have outweighed any differences in optimal bandwidths among each general approach.

The univariate LSCV generally was much better than the reference bandwidth method, but the univariate LSCV did have the most inconsistent performance of the LSCV options. In addition, it was most likely to have a global minimum different from the largest local minimum. For estimation of VI indices, using univariate options probably will change the VI scores only slightly. Univariate options did well at estimating home-range size at outer contours but performed badly at inner contours for combinations of 2 or 4 normals. Therefore, univariate approaches are a poor choice for estimating core areas.

The critical role of sample size on kernel performance has been reported previously (Seaman et al. 1999). Sample size had a bigger effect on kernel performance than choice of LSCV option in our study. However, choice of a general type of bandwidth selection method (e.g., LSCV vs. h_{ref}) has a major effect on kernel performance. In our study, increasing sample size from 50 to 150 lowered bias less than choosing an LSCV option instead of h_{ref}.

In the statistical literature, some researchers view LSCV as an inferior bandwidth selection method compared to second-generation methods such as "plug-in" approaches (Wand and Jones 1995, Jones et al. 1996). Both plug-in and LSCV methods estimate the "ideal" bandwidth, the value that minimizes error between the true and estimated distributions. With LSCV, an estimate of this error is minimized across a range of bandwidth values. Plug-in methods use an analytical equation to directly estimate the ideal bandwidth. This equation contains a function of the unknown true density. A pilot bandwidth is used to estimate this function, and the estimate is "plugged in" to the equation (Bowman and Azzalini 1997). Although LSCV has low bias, all options have high sampling variability. The LSCV score function may have no meaningful minimum, particularly for point patterns with tight clumps of points (Silverman 1986, Seaman et al. 1998). The LSCV method essentially fails in these cases. Plug-in methods have lower sampling variability than LSCV but may not perform as well when the true distribution has sharp peaks (Wand and Jones 1995). Research is needed in the context of home-range estimation to determine whether plug-in methods generally are superior to LSCV or are at least a useful alternative when LSCV fails.

We assume that home-range software programs use the scaling, global minimum version of LSCV, although this usually is not stated. Of these LSCV approaches, only the scaling method has been explicitly described in the ecological literature (Seaman and Powell 1996). Because the scaling method performed similar to or better than other variants overall, it is adequate as the default LSCV method. Although some programs discuss the numerical optimization method used, none explicitly state that they search for the largest local minimum rather than just the global minimum. This difference may be trivial for many data sets. As noted in previous studies (e.g., Seaman and Powell 1996), h_{ref} usually had higher bias in home-range size estimates than any LSCV option and should not be the default selection method.

Differences among LSCV options were low compared to differences among each of these options and the reference method. However, choice of LSCV options can still affect comparability of UD estimates among studies. We recommend that authors of home-range software packages make explicit which forms of the LSCV or other bandwidth selection methods are implemented in their programs. Researchers using kernel estimates of UDs should recognize the critical influence of bandwidth selection and understand the options offered or selected by default in their program of choice.

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