Bandwidth Selection and Reconstruction Quality in Point-Based Surfaces

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Abstract—We investigate the influence of bandwidth selection in the reconstruction quality of point-based surfaces. While the problem has received relatively little attention in the literature, we show that appropriate selection plays a significant role in the quality of reconstructed surfaces. We show how to compute optimal bandwidths for one class of moving-least squares surfaces by formulating the polynomial fitting step as a kernel regression problem for both noiseless and noisy data. In the context of Levin's projection, we also discuss the implications of the two-step projection for bandwidth selection. We show experimental comparisons of our method, which outperforms heuristically chosen functions and weights previously proposed. We also show the influence of bandwidth on the reconstruction quality of different formulations of point-based surfaces. We provide, to the best of our knowledge, the first quantitative comparisons between different MLS surface formulations and their optimal bandwidths. Using these experiments, we investigate the choice of effective bandwidths for these alternative formulations. We conclude with a discussion of how to effectively compare the different MLS formulations in the literature.

Index Terms—Bandwidth Selection, MLS Surfaces, Surface Reconstruction

1 INTRODUCTION

THERE has been a large, recent interest in the area of surface reconstruction from point-sampled data. This work has been motivated by a set of important applications where the ability to define continuous surfaces out of a set of discrete point samples is necessary. The resolution and availability of current 3-D range scanners that output a very large set of unconnected points has driven the development of effective techniques to reconstruct surfaces directly from the point cloud data.

One of the main challenges in effectively using these data is dealing with the inherently noisy and irregular nature of the acquired dataset. The noise introduced by these point-ofview scanners is dependent on factors such as the material of the object being reconstructed, incident angle of the rangefinder laser on the object, and distance to the scanner. This means there typically are different noise levels throughout the range scan, and reconstruction techniques must cope with these issues to be successful. Notably, these three-dimensional range scans are currently being used in digital archeology, where the acquired data is considered a historical artifact. In some of these scans, it is possible to recover details that elucidate the technique used by the artist [1]. It becomes very important, then, to recover as much detail as possible.

In particular, Moving Least-Squares surfaces [2], [3] have shown to be a powerful and popular surface reconstruction method. An MLS surface is defined by a point cloud P and a *projection operator* $f : \mathbb{R}^2 \to \mathbb{R}^2$, which takes a point r in the neighborhood of a C^{∞} surface S (the *MLS surface*), and returns a point $f(r) \in S$ close to r. The points in P might generally not be in S, but in the limit of increasing density of P, it can be shown that P converges to S geometrically and topologically [4], [5]. One of the main attractions of MLS is its natural resilience to noise. This is easily done by changing the *bandwidths* of the point samples — their influence radii, essentially.

We address the problem of accurately selecting bandwidths for different point-based surface formulations. In particular, we derive optimal bandwidths (in a sense which we will make precise later) that can be used in one popular movingleast square surface formulation. This paper is an extended version of our previous conference submission [6], where we derive our results based on Levin's MLS surface. There are, however, other popular point-based surface definitions. In addition to the work presented at the conference, we study the relation between the bandwidths and reconstruction quality of alternative point-based surface formulations. These new experiments suggest that different formulations have different optimal bandwidths and reconstruction qualities. To the best of our knowledge, this is the first quantitative comparison between different MLS surface formulations, and sheds light on their respective reconstruction abilities. In the remainder of the paper, we discuss the choice of bandwidth for some of these formulations. While we do not have counterparts for the theoretical results we first derive, we investigate whether the computed optima are effective for these other formulations. As we will show, it is possible to use the optimal bandwidths of Levin's MLS surfaces for Adamson and Alexa's surface with good results.

2 RELATED WORK

There have been many different proposed formulations of MLS surfaces. These include the projection operator of Levin and Alexa et al [2], [3] and its implicit surface formulation [7].

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Simplified versions with favorable computational requirements have also been proposed, usually derived in as a combination of weighted centroids and normal fields [8], [9]. Fleishman et al. presented extensions that increase the method's robustness to outliers while also introducing sharp features in the surface [10]. Zwicker et al. suggested the most popular variant of the *k*-nearest neighbor rule for bandwidth determination [11]. Shen et al. use an implicit variant of MLS surfaces that allow for normal constraints, and a weighting function that includes interpolatory constraints [12]

In this work, we use four different MLS formulations. The first two, and the ones for which we discuss and derive optimal bandwidth formulas, are based on Levin and Alexa et al.'s projection operator [3]. In this paper, we will call these Levin's MLS surface. We then compare the definition to Alexa and Adamson's implicit surface formulation [8] (which we will call Alexa's MLS surface).

While much work has gone into different MLS surface formulations, relatively little attention has been paid to choosing bandwidths for the surface projection. Adamson et al. [13] originally proposed extending their weighted-centroid formulation to incorporate elliptical kernels, allowing the samples to conform to the principal curvatures of the surface. They provide an argument for picking ellipsoidal kernels for clean samples, there is no discussion of the influence of noise in the anisotropy estimation. It is not clear, then, how to derive optimality criteria using those definitions. Lipman et al. show a tight error bound for the pointwise error in the MLS approximation formula [14]. They use this bound to numerically minimize the error for each projection. This mathematically sound approach outperforms heuristically chosen neighborhood sizes in accuracy. On the other hand, they depend on a search scheme that can be computationally costly. Dey and Sun [4] and Kolluri [5] propose using weight functions that take into account the estimated local feature size of the surface. This has the critical advantage of provable convergence to the right surface, but it involves computing the Voronoi diagram of a large set of points, which is computationally expensive.

Most of the papers in the literature provide different surface definitions (see, for example, the survey of Cheng et al. [15]). To the best of our knowledge, there have not been substantial comparisons between these methods in terms of ideal bandwidth choices and reconstruction quality under these bandwidths. Because of the sheer number of different formulations, we cannot hope to have a comprehensive account of all different formulations. Still, we believe the comparisons we present in Section 5 bring light on the relative merits of each projection.

3 COMPUTING OPTIMAL BANDWIDTHS

In this section, we first review Levin's MLS projection operator, (following the presentation in [16]) and, in particular, the polynomial fitting step. Then we will reformulate this second step as a kernel regression problem. This leads to the discussion of weight functions and optimal bandwidths for 2-D functional data, after which we move on to the generalization into 3-D data. Finally, we discuss how to incorporate the method into MLS projections.

Fig. 1. An overview of the MLS surface projection operator we use in this paper. (from [16])

3.1 Background

Given a set of input points $P = p_i \subset R^2$ and a point r to be projected on S, the MLS surface is defined in two steps. In the first step, we find a local approximating hyperplane H that minimizes a locally-weighted sum of squared distances from p_i to H. The weights are given as a function of the distance from the projection of r onto H (called q), as shown in Figure 1. The local plane $H = \{x | \langle n, x \rangle - D = 0, x \in \mathbb{R}^2\}, n \in$ $\mathbb{R}^2, ||n|| = 1$ is found by finding the plane that minimizes a certain functional:

$$\hat{H} = \operatorname{argmin}_{H} \sum_{i=1}^{N} \left(\langle n, p_i \rangle - D \right)^2 \theta_i(||p_i - q||)$$
(1)

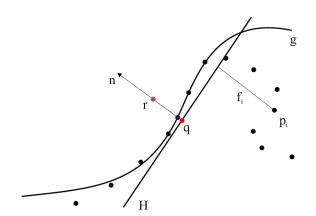
where θ is the weight function, the principal subject of this paper. After \hat{H} is found, a second step finds a local polynomial approximation \hat{g} of the surface, by minimizing a slightly different functional:

$$\hat{g} = \operatorname{argmin}_{g} \sum_{i=1}^{N} \left(g(x_{i}, y_{i}) - f_{i} \right)^{2} \theta_{i}(||p_{i} - q||)$$
(2)

where (x_i, y_i) are the representations of q_i , the projections of p_i onto \hat{H} expressed in the local coordinate system \hat{H} , and f_i is the signed height of p_i over \hat{H} . The same weighting functions are used, but notice that the weights now are not part of the optimization (q is fixed), so the optimization is linear. The most commonly used weighting function is a (possibly truncated) Gaussian:

$$w_h(r) = e^{-\frac{r^2}{h^2}}\chi_{[0,k)}(r)$$
(3)

k indicates a cutoff that is typically used for computational efficiency, limiting the distance query into the spatial data structures, and $\chi_{[a,b)}(x)$ is the function identically one if $a \leq x < b$, and zero otherwise. Although this function works well in practice, it is empirically chosen and little work has been done with respect to which weight functions are valid and which ones are optimal. In addition, this weight function has confined the shape of the neighborhood of the reference point to be isotropic, which might not be geometrically justified.



3.2 2-D Kernel Regression

We modify the problem setting to transform the interpolation problem into a regression problem. We use kernel regression because of the large amount of research that has been done into how to choose the weights appropriately. Kernel regression is conceptually very similar to weighted least-squares fitting. The statistical emphasis on expected errors allows us to define and compute optimal bandwidths. Additionally, these computations are elementary in nature: the only necessary machinery is a small amount of calculus. The basic idea is as follows: one writes the expression for the input points, the local regression function fit and the residuals, all as functions of the size (the bandwidth) of the selected kernel (typically a Gaussian). Then we simply take the derivative of the expected error, set it to zero, and solve for the bandwidth. The computations themselves become complicated because of the amount of terms that appear, but technically speaking they're straightforward.

To facilitate our discussion, we adopt the standard kernel regression terminology in statistics. Given random variables $X_1, ..., X_n$ with density g(X), response variables $Y_1, ..., Y_n$ that satisfy:

$$Y_i = f(X_i) + v^{1/2} \epsilon_i$$
, i = 1, ..., n

where v is the variance of the noise and ϵ_i are independent random variables for which

$$E(\epsilon_i | X_1, ..., X_n) = 0, Var(\epsilon_i | X_1, ..., X_n) = 1,$$

the value of f(x) at a specific point x is estimated by evaluating a polynomial p(t) of degree d at t = x. p(t) is defined as follows:

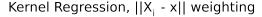
$$p(t) = \hat{\beta}_0 + \hat{\beta}_1(t-x) + \dots + \hat{\beta}_d(t-x)^d$$
(4)

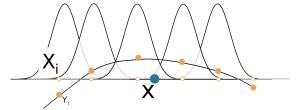
where $(\hat{\beta}_0, \hat{\beta}_1, ..., \hat{\beta}_d)$ minimizes

$$F(p) = \sum_{i=1}^{n} (Y_i - p(x))^2 K_h(X_i - x)$$
(5)

Here $K_h(u) = \frac{1}{h}K(\frac{u}{h})$ is a weight function (kernel) which assigns large weights to points within some neighborhood of x and small weights outside of the neighborhood. The size of neighborhood is controlled by parameter h. Notice that the weighting in kernel regression is a function of the distance between the values in the domain of the functional, $||X_i - x||$, while in MLS surfaces the weighting is a function of the distance between the actual samples and the center of the reference frame, $||p_i - q||$. This is illustrated in Figure 2.

The kernel function is usually chosen to be a symmetric and unimodal probability density function [17]. Common choices of kernels include the *normal kernel*, *Epanechnikov kernel* and *biweight kernel*. It has been proven [18] that in 2-D the bandwidth rather than the kernel plays the vital role in achieving high quality regression result. In other words, we can replace one kernel for another in regression without causing much loss of acuracy if we use the optimal bandwidth for each of them respectively. The Gaussian kernel we use is within 95% of the efficiency of the Epanechnikov kernel, the asymptotically optimal choice in the kernel regression setting. While these results only hold in the context of kernel





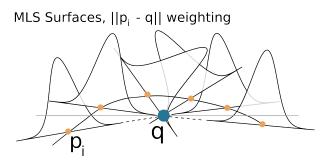


Fig. 2. Even though kernel regression and MLS surfaces both employ kernels, the way samples are weighted is different.

regression, they provide a justification for focusing in the bandwidth selection more than in the particular kernel shape.

In the following discussions of this paper, we will focus on two error criteria for the evaluation of performance of kernel regression: the first one is the Mean Squared Error (MSE) which emphasizes the expected error of the local specific point of interest:

$$MSE(p(x)) = (E[p(x) - f(x)])^2$$
(6)

and the other one is the integral of MSE over the functional domain which summarizes the overall expected errors:

$$\mathbf{MISE}(p(x)) = \int \mathbf{MSE}(x)g(x)dx \tag{7}$$

We have the following formula for MSE [19]:

$$\mathsf{MSE}(p(x)) \simeq \frac{1}{4} h^4 (f''(x))^2 \mu_2(K)^2 + \frac{R(K)v}{nhg(x)} \tag{8}$$

where

$$\mu_2(K) = \int z^2 K(z) dz, \quad R(K) = \int K^2(z) dz$$

The error term of MSE in Equation 8 is $o_P(n^{-1}h^{-1} + h^2)$. Letting the derivative of the approximated MSE be 0 and solving for h, we get the h that minimizes MSE:

$$h_{opt} = C \left(\frac{v}{ng(x)(f''(x))^2}\right)^{1/5}$$
(9)

where $C = (R(K)/\mu_2(K)^2)^{\frac{1}{5}}$ is a constant dependent on the kernel, e.g, for normal kernel $C = 1/(2\sqrt{\pi})^{\frac{1}{5}}$.

Computing the optimal bandwidth involves calculating g(x), f''(x) and v, which are determined by the underlying function, which is exactly the object we are trying to approximate. The standard solution to this problem is to settle for *estimators* of

these unknown values. We compute these estimators, and use them instead of the fundamentally impossible alternative of computing these functions over the unknown function. This is known in statistics as the "plug-in" method [20], [19], [21]. Among various ways to estimate the density g(x), we choose to use kernel density estimation because of its accuracy and close relation to kernel regression:

$$g(x) = \frac{1}{nh} \sum_{i=1}^{n} K\left(\frac{x - X_i}{h}\right)$$
(10)

Once again, we need to choose the right bandwidth. We are only looking for an unbiased estimator of g(x), so many choices are possible. We use the *normal scale rule* [18] to select the bandwidth:

$$h = \left(\frac{8\pi^{1/2}C}{3n}\right)^{1/5}\sigma\tag{11}$$

where C is defined as before and σ is the sample standard deviation. The intuition behind the normal scale rule is that

The normal scale rule essentially uses the optimal bandwidth for normal density as the bandwidth.

To estimate the second derivatives, we apply ordinary least squares quartic polynomial fitting to approximate the underlying functional. It has been shown [22] that it is necessary to divide the functional domain Ω into several "blocks" to make the method work for fast oscillating functionals. The "blocking method" divides the domain according to Mallow's C_p [23]. C_p is a statistic defined for the regression model of fitting each of the N blocks of data to a p-1 degree of polynomial. The optimal N is the one that minimizes C_p . Technically, N is chosen from the set $\{1, 2, ..., N_{max}\}$ to minimize:

$$C_p(N) = \frac{RSS(N)(n - pN_{max})}{RSS(N_{max})} - (n - 2pN)$$
(12)

In our case, since we fit data to a quartic polynomial, p = 5 and the C_p becomes:

$$C_p(N) = \frac{RSS(N)(n-5N_{max})}{RSS(N_{max})} - (n-10N)$$
(13)

where RSS(N) is the residual sum of squares over N blocks. In order to reduce the chance of overfitting, the following formula for N_{max} [19] has been suggested:

$$N_{max} = max\{min(\lfloor n/20 \rfloor, N^*), 1\}$$
(14)

where N^* is a user specified parameter which sets the upper limit of the number of blocks. As for variance, we use the estimator suggested by Ruppert et.al [19]:

$$v = \frac{RSS(N)}{n - 5N} \tag{15}$$

Assume $X_i \in [a, b]$, the optimal bandwidth based on MISE can be derived in an analogous way and the result is:

$$h_{opt} = C \left(\frac{v(b-a)}{n \int_{a}^{b} (f''(x))^2 g(x) dx} \right)^{1/5}$$
(16)

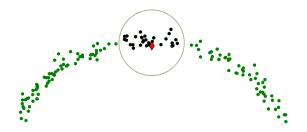


Fig. 3. Incorporating the kernel selector in MLS surfaces. A neighborhood around q (red diamond) is chosen among the sample data and kernel regression is applied to points within the neighborhood.

The only new difficulty that arises in the MISE based formula is estimation of the integral of the square of second derivative. We approximate the integral by Monte Carlo Integration:

$$\int_{\Omega} (f''(x))^2 g(x) dx \simeq \frac{b-a}{n} \sum_{i=1}^N \sum_{\{j: x_j \in \text{block } i\}} p''(x_j)^2 \quad (17)$$

3.3 3-D Kernel Regression

In 3-D space, we work on vectors $\mathbf{x} = (x_1, x_2)^T$ instead of scalars. The formulation of kernel regression problem in 3-D space is analogous to that in 2-D space except that the bandwidth *B* is now a matrix and the kernel function $K_B(\mathbf{x}) = |B|^{-1/2} K(B^{1/2}\mathbf{x})$. $K(\mathbf{x})$ can be constructed from a univarite kernel function in one of the two ways:

$$K(\mathbf{x}) = k(x_1)k(x_2) \text{ or } K(\mathbf{x}) = \frac{k((\mathbf{x}^T \mathbf{x})^{1/2})}{\int k((\mathbf{x}^T \mathbf{x})^{1/2})d\mathbf{x}}$$

If the univariate kernel is *normal*, we get the same bivariate Gaussian kernel in either way of construction:

$$K(\mathbf{x}) = \frac{1}{2\pi} e^{-\frac{1}{2}\mathbf{x}^T \mathbf{x}}$$
(18)

This property of Gaussian kernel motivates us to use it as our kernel function in the following discussions.

Different from 2-D kernel regression, the bandwidth matrix B not only controls the size of the neighborhood but also the shape. If B takes the following form:

$$\mathbf{B} = \begin{bmatrix} h^2 & 0\\ 0 & h^2 \end{bmatrix} \tag{19}$$

the shape of the neighborhood would be circular on the XY plane; if B is of the following form

$$\mathbf{B} = \begin{bmatrix} h_1^2 & 0\\ 0 & h_2^2 \end{bmatrix}$$
(20)

then the neighborhood on the XY plane is an ellipse with its axes parallel to the coordinate axes. The MSE for an arbitrary B [24] is:

$$MSE \simeq \frac{1}{4}\mu_2(K)^2 tr^2(\mathbf{B}\mathcal{H}_f(\mathbf{x})) + \frac{R(K)v}{ng(\mathbf{x})|\mathbf{B}|^{1/2}}$$
(21)

where

$$\mu_2(K)\mathbf{I} = \int \mathbf{z}\mathbf{z}^T K(\mathbf{z}) d\mathbf{z}, \ R(K) = \int K^2(\mathbf{z}) d\mathbf{z}$$

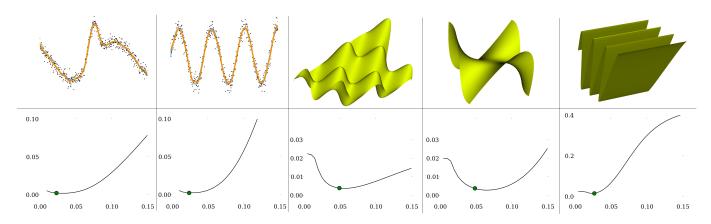


Fig. 4. Optimal bandwidths for 2-D and 3-D functional data, with circular kernels in the case of 3-D data. The underlying functionals are shown in Tables 1 and 2. The bottom row shows plots of bandwidth vs. Mean Squared Error. Our algorithm finds a value close to the real minimum in all cases.

 $\mathcal{H}_f(\mathbf{x})$ is the Hessian Matrix and $tr(\mathbf{B})$ is the trace of **B**. The error term of MSE in Equation (21) is $o_P\{n^{-1}|\mathbf{B}|^{-1/2} + tr^2(\mathbf{B})\}$.

To find the optimal bandwidths, we plug in a particular form of B into approximated MSE and try to find the minimizer. For circular kernel based on MSE we have:

$$h_{opt} = \left(\frac{2R(K)v}{n\mu_2(K)^2(\frac{\partial^2 f}{\partial x_1^2} + \frac{\partial^2 f}{\partial x_2^2})^2 g(\mathbf{x})}\right)^{1/6}$$
(22)

If we choose *h* based on MISE, then the optimal *h* is (Assume $X_i \in [a, b] \times [c, d]$.):

$$h_{opt} = \left(\frac{2R(K)v(b-a)(d-c)}{n\mu_2(K)^2 \int (\frac{\partial^2 f}{\partial x_1^2} + \frac{\partial^2 f}{\partial x_2^2})^2 g(\mathbf{x}) d\mathbf{x}}\right)^{1/6}$$
(23)

For elliptical kernel, let:

$$C_1 = \frac{R(K)v}{ng(x)}, C_2 = \mu_2(K)^2, d_1 = \frac{\partial^2 f}{\partial x_1^2}, d_2 = \frac{\partial^2 f}{\partial x_2^2}$$

When $d_1d_2 > 0$, the optimal h_1 and h_2 satisfy:

$$h_1^2 = \sqrt{\frac{d_2}{d_1}} \left(\frac{C_1}{2C_2 d_1 d_2}\right)^{\frac{1}{3}}$$
(24)

$$h_2^2 = \sqrt{\frac{d_1}{d_2}} \left(\frac{C_1}{2C_2 d_1 d_2}\right)^{\frac{2}{3}}$$
(25)

When $d_1d_2 < 0$, no minimizer exists for MSE. In this case, one can either choose to use the circular kernel or the MISE based optimal bandwidth matrix which satisfies:

$$h_1^2 = \left(\frac{I_3}{I_1}\right)^{1/4} \left(\frac{R(K)v(b-a)(d-c)}{n\mu_2(K)^2(\sqrt{I_1I_3}+I_2)}\right)^{1/3}$$
(26)

$$h_2^2 = \left(\frac{I_1}{I_3}\right)^{1/4} \left(\frac{R(K)v(b-a)(d-c)}{n\mu_2(K)^2(\sqrt{I_1I_3}+I_2)}\right)^{1/3}$$
(27)

where

$$I_1 = \int \left(\frac{\partial^2 f}{\partial x_1^2}\right)^2 g(\mathbf{x}) d\mathbf{x}$$
(28)

$$I_2 = \int \frac{\partial^2 f}{\partial x_1^2} \frac{\partial^2 f}{\partial x_2^2} g(\mathbf{x}) d\mathbf{x}$$
(29)

$$I_3 = \int \left(\frac{\partial^2 f}{\partial x_2^2}\right)^2 g(\mathbf{x}) d\mathbf{x}$$
(30)

and $X_i \in [a, b] \times [c, d]$.

As in 2-D, we approximate the underlying functional by ordinary quartic polynomial fitting. The integrals are approximated by Monte Carlo Integration and the densities are estimated by kernel density estimation with optimal bandwidth matrix $n^{-1/3}\Sigma$ (Σ is the sample covariance matrix) found again by the normal scale rule[25]. We also use the 3-D version of "blocking" method to adapt our method to fast-oscillating functionals.

In our formulas for optimal bandwidths, we found that the optimal bandwidths are proportional to variance of noise variable. This means that higher noise level motivates us to choose larger bandwidths. In addition, optimal bandwidths are inversely proportional to the number of samples, a quantity related to the curvature (second derivatives) and the density. This means that more samples, higher curvature or higher density all lead to smaller bandwidth. Our formulas agree with the intuition.

3.4 MLS

We have investigated two ways to incorporate our method into MLS. We first chose a neighborhood for each q which ensures that all points in that neighborhood are sampled from a functional instead of, say, double-sheeted surfaces, and then applied kernel regression using kernel regression weighting within that neighborhood (Figure 3); We also used kernel regression with MLS weighting on the whole dataset but this time we employed local weighted polynomial fitting to estimate the second derivatives of the underlying surfaces, etc. to find the optimal bandwidth.

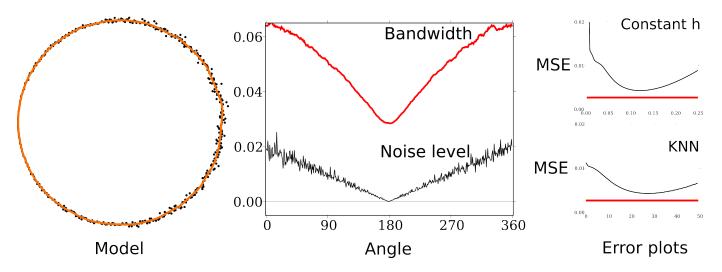


Fig. 5. MISE based circular kernel incoporated into *MLS*. We use as a model a circle with varying levels of noise (on the left). In the middle, the red line shows the selected bandwidth as a function of angle, and the black line shows the measured noise. On the right column, we show the results of choosing a constant h or a certain value of k for the k nearest neighbor heuristic. Notice that the optimal bandwidth around regions of no noise is not zero (see Section 6).

The advantage of the first method is that by simply using linear polynomial fitting, we can have a reconstruction whose precision is higher than heuristic approaches (Figure 6). Since it uses the kernel weighting scheme instead of the MLS weighting scheme (Figure 2), the distances between the sample points and underlying surface along the normal directions do not affect the weights assigned to each point. This helps reduce estimator bias: using MLS weighting, there is an inherent bias towards f(x) = 0. The non-trivial part of this method is how to choose a neighborhood for each q that quantantees all the points selected are sampled from a functional. We empirically chose the size of the neighborhood for q in our experiments. However, this choice is not critical: in places where the neighborhoods and reference frames are likely to not be functional, the MLS method will typically fail [26], [27].

As for the second method, there is no trouble of selecting a neighborhood for q. However, since Euclidean distances are used here, nonlinear regression instead of linear regression should be applied to alleviate the bias problem. It is comparatively easy to find optimal bandwidths for nonlinear polynomial fitting in 2-D [19], but we were unable to generalize the result to 3-D due to the complexity of the equation systems. We believe, however, that such a derivation is possible, and intend to pursue it in future work. In the following sections, we present experimental results using the first method.

4 EXPERIMENTAL RESULTS WITH LEVIN'S MLS

Since the second step of Levin's MLS is polynomial fitting on functional data, testing our methods on functional data is enough for evaluation their effectiveness. For completeness, however, we present experimental results of the method's performance after it is incorporated into MLS. To test our methods for functional data, we compared our results with the

Name	Function
F_1	$\sin(8x-4) + e^{-16(4x-2)^2}$
F_2	$sin(6.5\pi x)$

TABLE 1 2-D functionals in experiments

Name	Function
F_3	$0.3\cos(12x)\sin(9y) + e^{-\frac{9}{4}(x^2 + y^2)}$
F_4	$(2x-1)^3 - 3(2x-1)(2y-1)^2$
F_5	cos(20x)

TABLE 2 3-D functionals in experiments

real optimum; to test our methods in MLS, we compared our methods with heuristic approaches for bandwidth selection.

4.1 Functionals

For 2-D functionals, we tested our algorithm on points sampled from functions in Table 1. Sample size is 500 and the distribution of noises is N(0, 0.2). To evaluate the performance of the algorithm, we checked 100 possible values of the bandwidth from the interval [0, 1] and compared the integral squared error of the approximated curves using these bandwidths against the one produced by our algorithm. Figure 4 shows the comparison results. Our results are close to optimal, even in data sets with high noise level or fast oscillation.

For 3-D functionals, we chose to test MISE based circular kernel in the same setting as 2-D functionals. The underlying functionals are shown in Table 2. As in 2-D case, our reconstruction error is close to the real minimum (Figure 4).

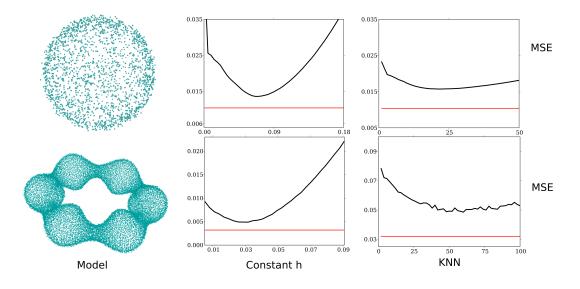


Fig. 6. MISE based circular kernel incorporated into MLS, using two synthetic models whose ground truth is known. The top model is a sphere, the bottom one an undulating torus, with varying inner radius. The middle column shows the mean squared error over the entire surface of varying h, and the right column shows the error using the k nearest neighbor heuristic. Our results are represented by the straight lines in the plots.

4.2 MLS

We have evaluated our method quantitatively reconstructing a circle (Figure 5), a sphere and an undulating torus with changing inner radius (Figure 6). In our evaluation, we compared our method against two commonly used heuristic approaches for bandwidth selection - a constant h for all projected points and the k-Nearest Neighbor method which uses a third of the distance from q to its kth nearest neighbor as the standard deviation of the Gaussian kernel. As in our experiments for functional data, we enumerated possible values of h and k and compared the reconstruction errors (distances between the reconstructed surface and real underlying surface) of different methods.

As demonstrated by the experimental results, our method outperforms the heuristic approaches. First, it is not clear how to find the optimal h or k for all possible projected points, while we have a closed-form analytical solution for a large family of cases. Second, and more importantly, the results show that there isn't a particular h or k that is best suited for the entire model, even in the case of constant noise. As we argue in Section 6, our method outperforms both algorithms because it makes fewer assumptions about the neighborhood configurations.

We also tested our method on real world models. Figure 8 shows that a visually acceptable reconstruction by heuristic approaches may fail to capture the geometry precisely, but our approach is capable of achieving close approximation to the real surface.

Since we used the first method of incorporating the kernel selectors into MLS, we had to choose a neighborhood for each q. The size of this neighborhood affects the quality of reconstruction but we've found that for a wide range of

neighbor sizes our method all produced reconstruction errors smaller than heuristic approaches. The neighborhoods used in the figures are not necessarily the best. For example, to reconstruct the circle (Figure 5), we set $(maxX_i - minX_i)/10$ as the neighborhood size but $(maxX_i - minX_i)/5$ produced better results. The important point, however, is that both of them significantly outperform the heuristic approaches.

Our bandwidth selector is fast. We tested the data for Figure 5 on an 2.8G Hz Linux machine with AMD Athlon(tm) 64 X2 Dual Core Processor 5600+. The second step (polynomial fitting) of MLS took a total of 8.917 seconds, among which 1.160 seconds were used to calculate the bandwidths. The time consumption of bandwidth computation is only 13% of the total time spent on the second step of MLS.

5 OTHER FORMULATIONS

In section 3, we show that Levin's MLS is well-suited to bandwidth analysis through kernel regression and derive several formulas for optimal bandwidths. Other moving leastsquares surface formulations exist, and are at least as popular as Levin's. In particular, formulations that use an implicit surface definition are very popular. Unfortunately, these are much harder with respect statistically in the fashion we have done above- we were unable to derive optimal bandwidth results for these. Because all these definitions are similar, one would expect the optimal bandwidths to be related to one another. If that were the case, one could compute optimal bandwidths with the formulas presented above and still use these alternative surface definitions. That is exactly what we will investigate in this section: the possibility of using our previous results in more general settings. Levin's MLS surface is only one of many equally popular surface definitions.

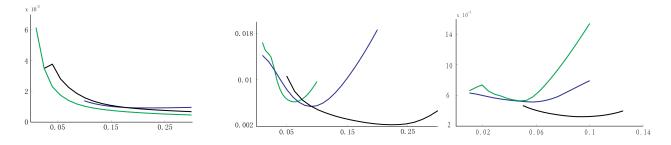


Fig. 7. Error curves of Alexa's and Levin's projection (bandwidth vs. reconstruction error). Levin's MLS with linear fitting is shown in green, Levin's MLS with quadratic fitting is shown in black, and Alexa's MLS is shown in blue. From left to right, the plots show reconstruction curves for a plane, a sphere and an undulating torus. In general, Alexa's MLS compares favorably to Levin's MLS with linear fitting, and unfavorably to the quadratic fitting version. See text for more details.

Alexa's MLS surface, in particular, is attractive because of implementation simplicity and performance. In this section, we study different MLS formulations and their behavior with changing bandwidths.

Different formulations of MLS have been proposed since the introduction of Levin's MLS. Given points $P = \{p_i \in R^3\}, i \in \{1, ..., N\}$, Alexa et. al define MLS surface implicitly as $S = \{\mathbf{x} \in \mathcal{B} | \mathbf{n}(\mathbf{x})^T (\mathbf{x} - \mathbf{a}(\mathbf{x}))\}$ where \mathcal{B} is a neighborhood containing surface S; $\mathbf{n}(\mathbf{x})$ is the normal at point x and $\mathbf{a}(\mathbf{x})$ is the weighted average of points at location x:

$$a(\mathbf{x}) = \frac{\sum_{i=1}^{N} \theta(||\mathbf{x} - \mathbf{p}_i||) \mathbf{p}_i}{\sum_{i=1}^{N} \theta(||\mathbf{x} - \mathbf{p}_i||)}$$

Several approaches for computing MLS surfaces based on Alexa et. al's formulation [8] have been introduced. One such approach is the "almost orthogonal projection" [8], which uses an iteration scheme to move x towards a(x) along n(x) until xconverges to a(x). Our implementation of Alexa's MLS uses this iteration.

We have performed experiments on three different analytical surfaces so we can measure reconstruction error. We have chosen to test these surfaces using a plane, a sphere, and the undulating torus described above. These choices were made because between the three models, we have surfaces with no curvature, positive gaussian curvature and negative gaussian curvature. The undulating torus features spatially changing curvature, which become important if we intend to gauge the adaptivity of a reconstruction method to changing surface features. For these three surfaces, we can compute the distance between a point and the surface, and so measure the quality of the reconstructions against the known ground truth.

Our experiments show curves of bandwidth versus reconstruction error in Figure 7. Another way to compute Alexa's MLS surfaces is to use n(a(q)) instead of n(q), as implemented in some PointShop3D plugins [28]. The advantage of using n(a(q)) is that it increases the size of the domain of points to be projected to the MLS surface. For reconstruction quality and bandwidth size, using n(a(q)) or n(q) generates undistinguishable results. Therefore, we only mention Alexa's MLS results, even though these are the same figures we get for the PointShop3D variation.

Figure 7 shows our experiments with different MLS formulations. We use a single bandwidth throughout the entire model, to compare the intrinsic reconstruction ability of each definition. With an optimal selector being used, we can expect better error curves, as evidenced in Figure 6. Our experimental results suggest that the optimal bandwidth of Alexa's projection yields better reconstruction quality than Levin's projection with linear fitting, but worse than Levin's projection with quadratic fitting. Additionally, it shows that the optimal bandwidth for Levin's linear fitting MLS is a reasonable (if slightly overfit) choice for optimal bandwidth in Alexa's MLS. The plane results merit some discussion: the linear version of Levin's MLS outperforms all the other formulations. This, however, only happens because the quadratic version of the operator "tries" to fit a quadratic through the noise, so it necessarily will suffer from overfitting. Notice that this does not happen on the other models.

The experiments provide favorable evidence for Alexa's MLS, which is much simpler than Levin's linear fitting MLS in formulation and implementation and arguably more robust, since each step does not involve non-linear optimizations. Even though the quadratic reconstruction can in theory generate better results, we could not derive formulas for the optimal bandwidth in those cases. We note that Alexa's MLS requires surface normals, of which we have assumed the presence. If that is not the case, then normals can be easily inferred from the covariance structure of the neighborhood. In our case, the normal field is computed as a weighted average of the normals, similar to what was suggested by Amenta and Kil [7]. Based on these results, we advocate the following heuristic for bandwidth selection when using Alexa's MLS surface: select the bandwidth with Levin's linear MLS as described previously, and increase the computed bandwidth by a small amount (15% or so).

It is also possible to interpret these experiments as evidence for the reconstruction quality obtained by Algebraic Point Set Surfaces [9]. That formulation has the distinction of incorporating both higher-order local surface fitting (by algebraic spherical fitting) and use of sample normals. These are the two features shared respectively by the quadratic version of Levin's MLS and Alexa's MLS. Unfortunately, that definition is much more complicated, and to the best of our knowledge,

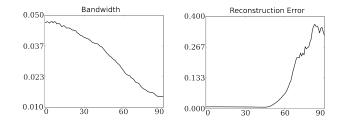


Fig. 9. Bandwidth and reconstruction error when the reference plane is rotated. Points are sampled from a circle with noise added. Left plot shows the bandwidth of a reference point when the rotation angle grows from 0 to 90 degrees; The right plot shows the reconstruction error associated with each reference point.

the current statistical tools are not sufficient to derive optimal bandwidth formulas.

6 DISCUSSION

In this section, we discuss issues such as the impact of this technique, its limitations, its applicability in other MLS surface definitions, and others.

Kernel regression weighting vs MLS surface weighting We use kernel regression weights (Figure2) to determine the optimal bandwidths, but use regular MLS weighting to actually perform the second step of polynomial fitting. While our experimental results clearly outperform the popular methods for choosing bandwidths, it is still important to investigate possible extensions of the optimal bandwidth derivations using MLS weighting.

Reconstruction quality It is interesting to reflect on the Mean Squared Error results we have obtained. At first glance, we might expect that for the case of i.i.d. noise there should exist a single h that performs as well as any algorithm. However, neighborhoods of i.i.d. samples are random variables themselves, so they are subject to variability. Then, across any particular model, there will be different optimal bandwidths. The k-nearest neighbor heuristic fails for similar reasons: it is effective at determining the local density of points, but not so at estimating whether the region is densely sampled or noisy. Figure 5 clearly illustrates this. The optimal bandwidth does not go to zero with the noise, which means that as the angle goes to 180, the algorithm is "shifting its focus" from noise to actual sampling density around the circle.

Kernel shapes induced by B We have derived optima for the class of diagonal matrices with positive eigenvalues, but it would be desirable to find a general solution for all symmetric positive-definite matrices. We have solved the equations, but they involve a system of several quadratic equations that we have currently been unable to solve. However, it is easy to circumvent this problem by rotating the coordinate system before computing the optimal bandwidths. This can be done by computing the *unweighted* covariance matrix of a neighborhood around q, and using the matrix of eigenvectors as a coordinate frame transformation. This will align the covariance axes with the coordinate frames, allowing the diagonal matrix to accurately capture the anisotropy. This works in general because all symmetric matrices are diagonalizable.

 $h \mapsto MISE(h)$ In some cases, we have observed the presence of more than one extrema in the function $h \mapsto MISE(h)$. While we have always observed a single minimum, we have occasionally seen maxima of the function. While it remains to be investigated under what conditions the function will have multiple extrema, in our experiments, the computed value of h is always extremely close to the minimum.

Bandwidths for the first step Recall that the MLS surface definition is based on a two-step approach. In current practice, the same bandwidths are used for both steps, but there's no particular reason for that decision. Perhaps the most interesting aspect of the results we have encountered is that the optimal bandwidths for the second step are significantly narrower than the bandwidths necessary for finding an appropriate reference frame. This means, essentially, that typical current MLS definitions tend to oversmooth the surfaces. A notable exception is the work of Pauly et al. [30], where Gaussian noise becomes a convolution of the relevant functions with the exact same noise distribution.

Nonlinear kernel regression We have been able to find the optimal bandwidth selector for nonlinear kernel regression in MLS in 2-D, but the derivation of optimal bandwidths for nonlinear kernel regression in 3-D is highly non-trivial [24]. In addition, the bandwidth selector for nonlinear kernel regression requires higher order derivative estimation, the accuracy of which is jeopardized by error propagation of numerical errors. In 2-D, a few steps of iteration is usually necessary to guarantee the precision of reconstruction [18].

Robustness of Levin's MLS surface fitting First is that it is possible to determine a good planar fit for the first step of Levin's MLS projection. Because the kernel regression setting requires a reference frame in which the data is representable as a function, if it is impossible to find an appropriate such first step, the results of kernel regression will not necessarily return a good fit. Levin's projection has been shown to have robustness issues in some settings [26], and this work does not try to solve these issues. We are interested in finding the best reconstruction quality at some point, *given that it is possible* to succesfully use Levin's projection.

Robustness of bandwidth selectors Our bandwidth selector is not integrated with the nonlinear optimization of MLS surfaces. To test the robustness of the method against imperfectly selected reference frames, we rotate the reference plane from 0 to 90 degrees and investigate the behavior of our bandwidth selectors. As shown in Figure 9, the bandwidth selector are capable of selecting bandwidth adaptively according to the local neighborhood up to 45 degrees - the bandwidths change with rotation angles while the reconstruction errors stay at the same level. This means our bandwidth selectors are insensitive to possible errors in the first step. In addition, the curve that plots bandwidth against angle approximates a cosine curve, which agrees with the fact that when the reference plane is rotated by angle θ approximately only $cos(\theta)$ of the original points remain in the neighborhood.

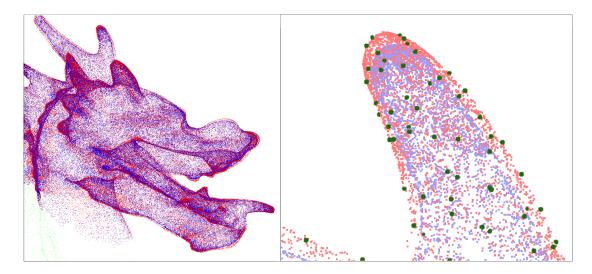


Fig. 8. Dragon head reconstructed from points sampled by afront [29] of the dragon model in the Stanford Scanning Model Repository. Red points are projections of reference points using our MISE-based kernel selector; blue points are projections using a constant bandwidth across the point set. Red points are close to real surface (green points) while the surface composed of blue points contracts.

7 CONCLUSION AND FUTURE WORK

In this paper, we study the relation between bandwidth selection and reconstruction quality for point-based surfaces. We provide a solid theoretic foundation for choosing bandwidths in polynomial fitting step in the MLS procedure. We discuss the possible choices of weight functions and we propose algorithms for choosing the optimal parameters for weight functions. We have tested our methods on functionals, surfaces and real world scanning models. Our methods work for clean data as well as for noisy data.

We then use these techniques as a basis for comparing different point-based surface representations, and suggest bandwidth selection techniques for cases where analytical formulas are otherwise unavailable. To the best of our knowledge, this is the first work that provides quantitative comparisons between these popular surface definitions.

We are currently working on generalizing the kernel selector for higher degree polynomial fitting from 2-D to 3-D. In some cases it might be desirable to settle for numerical optimization, using nonlinear optimizers such as conjugate gradients to explicitly minimize the MISE instead of analytically deriving the optimal value.

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APPENDIX

In this section, we provide the derivation for optimal bandwidth formulas in 3-D.

Circular Kernel

By Equation (21) we have:

$$MSE \simeq \frac{\mu_2(K)^2 h^4}{4} \left(\frac{\partial^2 f}{\partial x_1^2} + \frac{\partial^2 f}{\partial x_2^2}\right)^2 + \frac{R(K)v}{nh^2 g(\mathbf{x})}$$
(31)

By setting MSE' to be 0 and solving the equation, we obtain the optimal h:

$$h_{opt} = \left(\frac{2R(K)v}{n\mu_2(K)^2(\frac{\partial^2 f}{\partial x_1^2} + \frac{\partial^2 f}{\partial x_2^2})^2 g(\mathbf{x})}\right)^{1/6}$$
(32)

If we choose h based on MISE:

$$\text{MISE} \simeq \frac{\mu_2(K)^2 h^4}{4} \int (\frac{\partial^2 f}{\partial x_1^2} + \frac{\partial^2 f}{\partial x_2^2})^2 g(\mathbf{x}) d\mathbf{x} + \frac{R(K)v}{nh^2}$$
(33)

then the optimal h is:

$$h_{opt} = \left(\frac{2R(K)v}{n\mu_2(K)^2 \int (\frac{\partial^2 f}{\partial x_1^2} + \frac{\partial^2 f}{\partial x_2^2})^2 g(\mathbf{x}) d\mathbf{x}}\right)^{1/6}$$
(34)

Elliptical Kernel

By Equation (21) we have:

$$MSE \simeq \frac{\mu_2(K)^2}{4} (h_1^2 \frac{\partial^2 f}{\partial x_1^2} + h_2^2 \frac{\partial^2 f}{\partial x_2^2})^2 + \frac{R(K)v}{nh_1h_2g(\mathbf{x})}$$
(35)

To simplify demonstration of our derivation, let:

$$C_1 = \frac{R(K)v}{ng(x)}, C_2 = \mu_2(K)^2, d_1 = \frac{\partial^2 f}{\partial x_1^2}, d_2 = \frac{\partial^2 f}{\partial x_2^2}$$

then MSE can be rewritten as

$$MSE = \frac{C_1}{h_1 h_2} + \frac{C_2}{4} (d_1 h_1^2 + d_2 h_2^2)^2$$
(36)

Now we have:

$$\frac{\partial \text{MSE}}{\partial h_1} = -\frac{C_1}{h_1^2 h_2} + C_2 d_1 h_1 (d_1 h_1^2 + d_2 h_2^2) \quad (37)$$

$$\frac{\partial \text{MSE}}{\partial h_2} = -\frac{C_1}{h_1 h_2^2} + C_2 d_2 h_2 (d_1 h_1^2 + d_2 h_2^2) \quad (38)$$

When $d_1d_2 > 0$, by setting both equations to be 0 we get:

$$h_1^2 = \sqrt{\frac{d_2}{d_1}} \left(\frac{C_1}{2C_2 d_1 d_2}\right)^{1/3}$$
(39)

$$h_2^2 = \sqrt{\frac{d_1}{d_2}} \left(\frac{C_1}{2C_2 d_1 d_2}\right)^{1/3} \tag{40}$$

When $d_1d_2 < 0$, no minimizer exists for MSE: If $d_1(d_1h_1^2 + d_2h_2^2) < 0$, then $\frac{\partial MSE}{\partial h_1} < 0$ for $\forall h_1$; if $d_1(d_1h_1^2 + d_2h_2^2) > 0$, then $\frac{\partial MSE}{\partial h_2} < 0$ for $\forall h_2$. In this case, one can either choose to use the circular kernel or the MISE based optimal bandwidth matrix. By analogous analysis, the optimal h_1 and h_2 based on MISE satisfy:

$$h_1^2 = \left(\frac{I_3}{I_1}\right)^{1/4} \left(\frac{R(K)v}{n\mu_2(K)^2(\sqrt{I_1I_3} + I_2)}\right)^{1/3}$$
(41)

$$h_2^2 = \left(\frac{I_1}{I_3}\right)^{1/4} \left(\frac{R(K)v}{n\mu_2(K)^2(\sqrt{I_1I_3}+I_2)}\right)^{1/3}$$
(42)

where

$$I_1 = \int \left(\frac{\partial^2 f}{\partial x_1^2}\right)^2 g(\mathbf{x}) d\mathbf{x}$$
(43)

$$I_2 = \int \frac{\partial^2 f}{\partial x_1^2} \frac{\partial^2 f}{\partial x_2^2} g(\mathbf{x}) d\mathbf{x}$$
(44)

$$I_3 = \int \left(\frac{\partial^2 f}{\partial x_2^2}\right)^2 g(\mathbf{x}) d\mathbf{x}$$
(45)

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