

¹ This is a draft version of work in progress, content will be revisited in subsequent versions.

² **Robust Local Polynomial Regression with Similarity Kernels**

³ Yaniv Shulman

⁴ *yaniv@shulman.info*

⁵ **Abstract**

Local polynomial regression is a powerful and flexible statistical technique that has gained increasing popularity in recent years due to its ability to model complex relationships between variables. Local polynomial regression generalizes the polynomial regression and moving average methods by fitting a low-degree polynomial to a nearest neighbors subset of the data at the location. The polynomial is fitted using weighted ordinary least squares, giving more weight to nearby points and less weight to points further away. Local polynomial regression is however susceptible to outliers and high leverage points which may cause an adverse impact on the estimation accuracy. The main contribution of this paper is to revisit the kernel that is used to produce local regression weights. The simple yet effective idea is to generalize the kernel such that both the predictor and the response are used to calculate weights. Within this framework, two positive definite kernels are proposed that assign robust weights to mitigate the adverse effect of outliers in the local neighborhood by estimating and utilizing the density at the local locations. The method is implemented in the Python programming language and is made publicly available at <https://github.com/yaniv-shulman/rsklpr>. Experimental results on synthetic benchmarks across a range of settings demonstrate that the proposed method achieves competitive results and generally improves on the standard local polynomial regression method.

6 **1. Introduction**

7 Local polynomial regression (LPR) is a powerful and flexible statistical technique that has
8 gained increasing popularity in recent years due to its ability to model complex relationships be-
9 tween variables. Local polynomial regression generalizes the polynomial regression and moving
10 average methods by fitting a low-degree polynomial to a nearest neighbors subset of the data at
11 the location. The polynomial is fitted using weighted ordinary least squares, giving more weight
12 to nearby points and less weight to points further away. The value of the regression function for
13 the point is then obtained by evaluating the fitted local polynomial using the predictor variable
14 value for that data point. LPR has good accuracy near the boundary and performs better than all
15 other linear smoothers in a minimax sense [2]. The biggest advantage of this class of methods
16 is not requiring a prior specification of a function i.e. a parametrized model. Instead only a
17 small number of hyperparameters need to be specified such as the type of kernel, a smoothing
18 parameter and the degree of the local polynomial. The method is therefore suitable for modeling
19 complex processes such as non-linear relationships, or complex dependencies for which no the-
20 oretical models exist. These two advantages, combined with the simplicity of the method, makes
21 it one of the most attractive of the modern regression methods for applications that fit the general
22 framework of least squares regression but have a complex deterministic structure.

23 Local polynomial regression incorporates the notion of proximity in two ways. The first is
24 that a smooth function can be reasonably approximated in a local neighborhood by a simple
25 function such as a linear or low order polynomial. The second is the assumption that nearby
26 points carry more importance in the calculation of a simple local approximation or alternatively
27 that closer points are more likely to interact in simpler ways than far away points. This is achieved
28 by a kernel which produces values that diminish as the distance between the explanatory variables
29 increase to model stronger relationship between closer points.

30 Methods in the LPR family include the Nadaraya-Watson estimator [10, 18] and the estimator
31 proposed by Gasser and Müller [7] which both perform kernel based local constant fit. These
32 were improved on in terms of asymptotic bias by the proposal of the local linear and more general
33 local polynomial estimators [16, 3, 9, 4, 5]. For a review of LPR methods the interested reader
34 is referred to [2].

35 LPR is however susceptible to outliers, high leverage points and functions with discontinu-
36 ities in their derivative which often cause an adverse impact on the regression due to its use
37 of least squares based optimization [17]. The use of unbounded loss functions may result in
38 anomalous observations severely affecting the local estimate. Substantial work has been done to
39 develop algorithms to apply LPR to difficult data. To alleviate the issue [15] employs variable
40 bandwidth to exclude observations for which residuals from the resulting estimator are large. In
41 [3] an iterated weighted fitting procedure is proposed that assigns in each consecutive iteration
42 smaller weights to points that are farther then the fitted values at the previous iteration. The pro-
43 cess repeats for a number of iterations and the final values are considered the robust parameters
44 and fitted values. An alternative common approach is to replace the squared prediction loss by
45 one that is more robust to the presence of large residuals by increasing more slowly or a loss that
46 has an upper bound such as the Tukey or Huber loss. These methods however require specifying
47 a threshold parameter for the loss to indicate atypical observations or standardizing the errors
48 using robust estimators of scale [8]. For a recent review of robust LPR and other nonparametric
49 methods see [17, 11]

50 The main contribution of this paper is to revisit the kernel used to produce regression weights.
51 The simple yet effective idea is to generalize the kernel such that both the predictor and the re-

52 response are used to calculate weights. Within this framework, two positive definite kernels are
 53 proposed that assign robust weights to mitigate the adverse effect of outliers in the local neighborhood by estimating the density of the response at the local locations. Note the proposed
 54 framework does not preclude the use of robust loss functions, robust bandwidth selectors and
 55 standardization techniques. In addition the method is implemented in the Python programming
 56 language and is made publicly available. Experimental results on synthetic benchmarks demon-
 57 strate that the proposed method achieves competitive results and generally performs better than
 58 LOESS/LOWESS using only a single training iteration.

60 The remainder of the paper is organized as follows: In section 2, a brief overview of the
 61 mathematical formulation of local polynomial regression is provided. In section 3, a framework
 62 for robust weights as well as specific robust positive definite kernels are proposed. In section
 63 5, implementation notes and experimental results are provided. Finally, in section 6, the paper
 64 concludes with directions for future research.

65 2. Local polynomial regression

66 This section provides a brief overview of local polynomial regression and establishes the no-
 67 tation subsequently used. Let (X, Y) be a random pair and $\mathcal{D}_T = \{(X_i, Y_i)\}_{i=1}^T \subseteq \mathcal{D}$ be a training
 68 set comprising a sample of T data pairs. Suppose that $(X, Y) \sim f_{XY}$ a continuous density and
 69 $X \sim f_X$ the marginal distribution of X . Let $Y \in \mathbb{R}$ be a continuous response and assume a model
 70 of the form $Y_i = m(X_i) + \epsilon_i$, $i \in 1, \dots, T$ where $m(\cdot) : \mathbb{R}^d \rightarrow \mathbb{R}$ is an unknown function and ϵ_i
 71 are independently distributed error terms having zero mean representing random variability not
 72 included in X_i such that $\mathbb{E}[Y|X=x] = m(x)$. There are no global assumptions about the function
 73 $m(\cdot)$ other than that it is smooth and that locally it can be well approximated by a low degree
 74 polynomial as per Taylor's theorem. Local polynomial regression is a class of nonparametric re-
 75 gression methods that estimate the unknown regression function $m(\cdot)$ by combining the classical
 76 least squares method with the versatility of non-linear regression. The local p -th order Taylor
 77 expansion for $x \in \mathbb{R}$ near a point X_i yields:

$$m(X_i) \approx \sum_{j=0}^p \frac{m^{(j)}(x)}{j!} (x - X_i)^j := \sum_{j=0}^p \gamma_j(x)(x - X_i)^j \quad (1)$$

78 To find an estimate $\hat{m}(x)$ of $m(x)$ the low-degree polynomial (1) is fitted to the N nearest neighbors
 79 using weighted least squares such to minimize the empirical loss $\mathcal{L}_{lpr}(\cdot; \mathcal{D}_N, h)$:

$$\mathcal{L}_{lpr}(x; \mathcal{D}_N, h) := \sum_{i=1}^N \left(Y_i - \sum_{j=0}^p \gamma_j(x)(x - X_i)^j \right)^2 K_h(x - X_i) \quad (2)$$

$$\hat{\gamma}(x) := \min_{\gamma(x)} \mathcal{L}_{lpr}(x; \mathcal{D}_N, h) \quad (3)$$

80 Where $\gamma, \hat{\gamma} \in \mathbb{R}^{p+1}$; $K_h(\cdot)$ is a scaled kernel, $h \in \mathbb{R}_{>0}$ is the bandwidth parameter and $\mathcal{D}_N \subseteq \mathcal{D}_T$
 81 is the subset of N nearest neighbors of x in the training set where the distance is measured on
 82 the predictors only. Having computed $\hat{\gamma}(x)$ the estimate of $\hat{m}(x)$ is taken as $\hat{\gamma}(x)_1$. Note the

83 term kernel carries here the meaning typically used in the context of nonparametric regression
 84 i.e. a non-negative real-valued weighting function that is typically symmetric, unimodal at zero,
 85 integrable with a unit integral and whose value is non-increasing for the increasing distance
 86 between the X_i and x . Higher degree polynomials and smaller N generally increase the variance
 87 and decrease the bias of the estimator and vice versa [2]. For derivation of the local constant and
 88 local linear estimators for the multidimensional case see [6].

89 3. Robust weights with similarity kernels

90 The main idea presented is to generalize the kernel function used in equation (2) to produce
 91 robust weights. This is achieved by using a similarity kernel function defined on the data domain
 92 $K_{\mathcal{D}} : \mathcal{D}^2 \rightarrow \mathbb{R}_+$ that enables weighting each point and incorporating information on the data in
 93 the local neighborhood in relation to the local regression target.

$$\mathcal{L}_{rsk}(x, y; \mathcal{D}_N, H) := \sum_{i=1}^N \left(Y_i - \sum_{j=0}^p \beta_j(x, y)(x - X_i)^j \right)^2 K_{\mathcal{D}}((x, y), (X_i, Y_i); H) \quad (4)$$

$$\hat{\beta}(x, y; \mathcal{D}_N, H) := \min_{\beta(x, y)} \mathcal{L}_{rsk}(x, y; \mathcal{D}_N, H) \quad (5)$$

94 Where H is the set of bandwidth parameters. There are many possible choices for such a
 95 similarity kernel to be defined within this general framework. However, used as a local weighting
 96 function, such a kernel should have the following attributes:

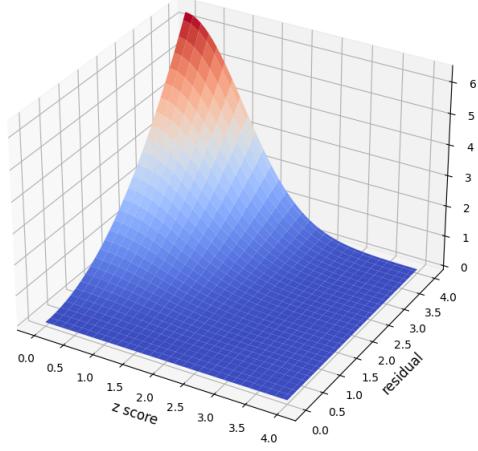
- 97 1. Non-negative, $K_{\mathcal{D}}((x, y), (x', y')) \geq 0$.
- 98 2. Symmetry in the inputs, $K_{\mathcal{D}}((x, y), (x', y')) = K_{\mathcal{D}}((x', y'), (x, y))$.
- 99 3. Tending toward decreasing as the distance in the predictors increases. That is, given a
 100 similarity function on the response $s(\cdot, \cdot) : \mathbb{R}^2 \rightarrow \mathbb{R}_+$, if $s(y, y')$ indicates high similarity
 101 the weight should decrease as the distance between the predictors grows, $s(y, y') > \alpha \implies$
 102 $K_{\mathcal{D}}((x, y), (x + u, y')) \geq K_{\mathcal{D}}((x, y), (x + v, y')) \quad \forall \|u\| \leq \|v\|$ and some $\alpha \in \mathbb{R}_+$.

103 In this work two such useful positive definite kernels are proposed. Similarly to the usual
 104 kernels used in (2), these tend to diminish as the distance between the explanatory variables
 105 increases to model stronger relationship between closer points. In addition, the weights produced
 106 by the kernels also model the "importance" of the pair (x, y) . This is useful for example to down-
 107 weight outliers to mitigate their adverse effect on the ordinary least square based regression.
 108 Formally let $K_{\mathcal{D}}$ be defined as:

$$K_{\mathcal{D}}((x, y), (x', y'); H_1, H_2) = K_1(x, x'; H_1)K_2((x, y), (x', y'); H_2) \quad (6)$$

109 Where $K_1 : \mathbb{R}^d \times \mathbb{R}^d \rightarrow \mathbb{R}_+$ and $K_2 : \mathcal{D}^2 \rightarrow \mathbb{R}_+$ are positive definite kernels and H_1, H_2 are
 110 the sets of bandwidth parameters. The purpose of K_1 is to account for the distance between a
 111 neighbor to the local regression target and therefore may be chosen as any of the kernel functions
 112 that are typically used in equation (2). The role of K_2 is described now in more detail as this
 113 is the main idea proposed in this work. Using K_2 , the method performs robust regression by
 114 detecting local outliers in an unsupervised manner and assigns them with lower weights. There
 115 are many methods that could be employed to estimate the extent to which a data point is a local
 116 outlier however in this work it is estimated in one of the following two ways.

Figure 1: Loss function, assuming a standard quadratic function of the residual, a standard normal density for K_2 and excluding the K_1 distance kernel scaling.



¹¹⁷ *Conditional density*

The first proposed method for K_2 is proportional to the estimated localized conditional marginal distribution of the response variable at the location:

$$K_2((x, y), (x', y'); H_2) = \hat{f}(y | x; H_2)\hat{f}(y' | x'; H_2) \quad (7)$$

The nonparametric conditional density estimation is performed using the Parzen–Rosenblatt window (kernel density estimator):

$$\hat{f}(y | x; H_2) = \hat{f}(x, y; H_2)/\hat{f}(x; H_2) \quad (8)$$

$$= \hat{f}(v; \mathbf{H}_v)/\hat{f}(x; \mathbf{H}_x) \quad (9)$$

$$= \frac{|\mathbf{H}_v|^{1/2} \sum_{i=1}^N K_v(\mathbf{H}_v^{-1/2}(v - V_i))}{|\mathbf{H}_v|^{1/2} \sum_{i=1}^N K_x(\mathbf{H}_x^{-1/2}(x - X_i))} \quad (10)$$

¹¹⁸ Where $v = [x, y] \in \mathbb{R}^{d+1}$ is the concatenated vector of the predictors and the response; and $\mathbf{H}_v, \mathbf{H}_x$
¹¹⁹ are bandwidth matrices.

¹²⁰ *Joint density*

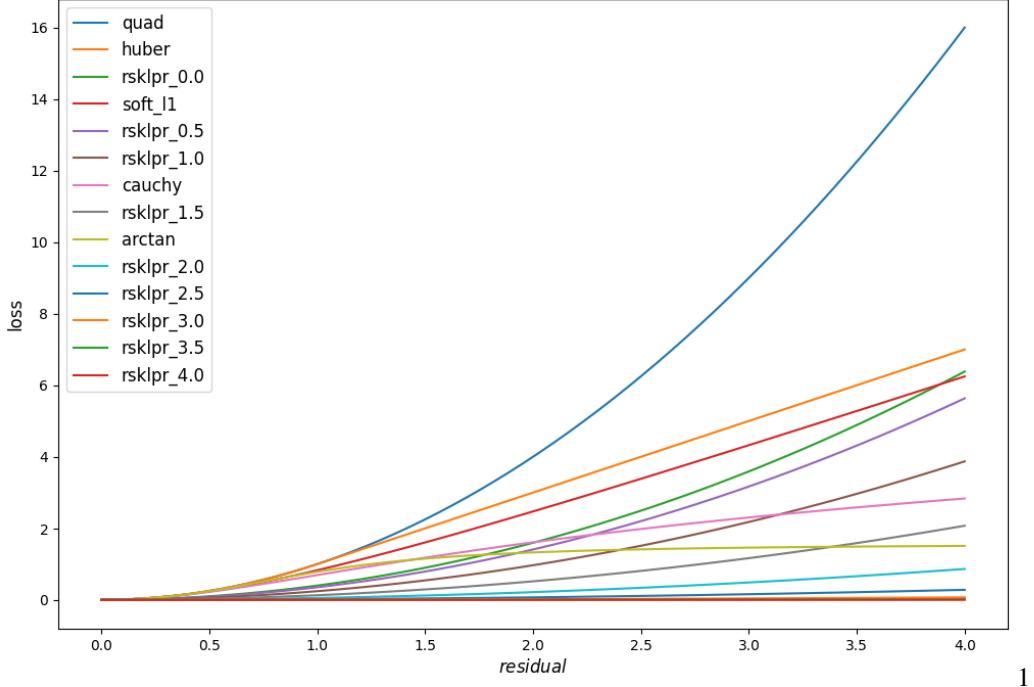
The second proposed kernel is proportional to the joint distribution of the random pair, this could be useful for example to also down-weight high leverage points:

$$K_2((x, y), (x', y'); H_2) = \hat{f}(x, y; H_2)\hat{f}(x', y'; H_2) \quad (11)$$

¹²¹ Where the joint density can be estimated using the same aforementioned approach.

¹²²

Figure 2: The plot illustrates the proposed loss function, a number of common robust losses and the standard quadratic residual loss for comparison. It is assumed that that K_2 is equivalent to the standard normal density and the K_1 distance kernel scaling is excluded. The numbers appended to "rsklpr" indicate how many standard deviations away from the mean the density is calculated. It is evident that the loss is heavily attenuated in regions of low density.



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123 Regardless of the choice of kernel, the hyperparameters of this model are similar in essence
 124 to the standard local polynomial regression and comprise the span of included points, the kernels
 125 and their associated bandwidths. Note that this estimator can be replaced with other robust
 126 density estimators and better results are anticipated by doing so however exploring this option is
 127 left for future work.

128 **4. Properties**

129 This section discusses some properties of the estimator. Note the notation in this section is
 130 simplified by excluding explicit mentions of D_N and H , however the analysis is conditional on
 131 the nearest neighbors in the sample, D_N .

132 *4.1. Invariance to y at the regression location and simplification of the objective*

133 The objective (5) is invariant to the value of y at the location (x, y) for the proposed similarity
 134 kernels.

135 *Proof:* The optimization is invariant to the scale of the objective function. Therefore:

$$\hat{\beta}(x, y) := \min_{\beta(x,y)} \sum_{i=1}^N \left(Y_i - \sum_{j=0}^p \beta_j(x, y)(x - X_i)^j \right)^2 K_{H_1}(x - X_i) \hat{f}(x, y) \hat{f}(X_i, Y_i) \quad (12)$$

$$= \sum_{i=1}^N \left(Y_i - \sum_{j=0}^p \beta_j(x, y)(x - X_i)^j \right)^2 K_{H_1}(x - X_i) \hat{f}(X_i, Y_i) \quad (13)$$

¹³⁶ The equality holds because $\hat{f}(x, y)$ is a constant scalar that uniformly scales the weights.
¹³⁷ Since the objective is now independent of y , it follows that:

$$\hat{\beta}(x, y) := \min_{\beta(x)} \sum_{i=1}^N \left(Y_i - \sum_{j=0}^p \beta_j(x)(x - X_i)^j \right)^2 K_{H_1}(x - X_i) \hat{f}(X_i, Y_i) \quad (14)$$

$$:= \hat{\beta}(x) \quad \forall y \quad (15)$$

¹³⁸ This simplification enables more efficient calculations of the estimator because the dependence
¹³⁹ on y is removed from the objective function. Note that $\hat{f}(X_i, Y_i)$ can also be replaced with
¹⁴⁰ $\hat{f}(Y_i | X_i)$ with similar results.

¹⁴¹ 4.2. Weighted arithmetic mean of the standard LPR

¹⁴² The proposed estimator is equivalent to the weighted arithmetic mean of the terms in the
¹⁴³ standard LPR loss (2), with weights $w_i = \hat{f}(X_i, Y_i)$.

¹⁴⁴ *Proof:* Since the optimization is invariant to scaling, we have:

$$\hat{\beta}(x) := \min_{\beta(x)} \sum_{i=1}^N \left(Y_i - \sum_{j=0}^p \beta_j(x)(x - X_i)^j \right)^2 K_{H_1}(x - X_i) \hat{f}(X_i, Y_i) \quad (16)$$

$$= \min_{\beta(x)} \left(\sum_{i=1}^N \hat{f}(X_i, Y_i) \right)^{-1} \sum_{i=1}^N \left(Y_i - \sum_{j=0}^p \beta_j(x)(x - X_i)^j \right)^2 K_{H_1}(x - X_i) \hat{f}(X_i, Y_i) \quad (17)$$

$$= \min_{\beta(x)} \left(\sum_{i=1}^N w_i \right)^{-1} \sum_{i=1}^N \left(Y_i - \sum_{j=0}^p \beta_j(x)(x - X_i)^j \right)^2 K_{H_1}(x - X_i) w_i \quad (18)$$

¹⁴⁵ The normalization by $\sum_{i=1}^N w_i$ shows the equivalence to the weighted arithmetic mean, with
¹⁴⁶ the weights $w_i = \hat{f}(X_i, Y_i)$.

¹⁴⁷ 4.3. Asymptotic degeneration of the estimator to the standard LPR

¹⁴⁸ Asymptotically, the proposed estimator degenerates to the standard LPR when the weights
¹⁴⁹ w_i are uncorrelated with the standard LPR terms. Formally, as $N \rightarrow \infty$, $\hat{\beta}(x) \rightarrow \hat{\gamma}(x)$, where
¹⁵⁰ $\hat{\gamma}(x)$ is the standard LPR estimator, and the condition that $\left(Y - \sum_{j=0}^p \beta_j(x)(x - X)^j \right)^2 K_{H_1}(x - X)$

¹⁵¹ and $\hat{f}(X, Y)$ are uncorrelated holds. It is assumed that (X_i, Y_i) are independent and identically
¹⁵² distributed (i.i.d.) random variables and that $\hat{f}(X, Y) > 0$ almost everywhere.

¹⁵³ *Proof:* Define

$$g(X, Y) := \left(Y - \sum_{j=0}^p \beta_j(x)(x - X)^j \right)^2 K_{H_1}(x - X),$$

it follows that:

$$\hat{\beta}(x) := \min_{\beta(x)} \left(\sum_{i=1}^N \hat{f}(X_i, Y_i) \right)^{-1} \sum_{i=1}^N g(X_i, Y_i) \hat{f}(X_i, Y_i) \quad (19)$$

$$= \min_{\beta(x)} \left(\frac{1}{N} \sum_{i=1}^N \hat{f}(X_i, Y_i) \right)^{-1} \left(\frac{1}{N} \sum_{i=1}^N g(X_i, Y_i) \hat{f}(X_i, Y_i) \right) \quad (20)$$

As $N \rightarrow \infty$, by the law of large numbers, we obtain:

$$\left(\frac{1}{N} \sum_{i=1}^N \hat{f}(X_i, Y_i) \right)^{-1} \xrightarrow{a.s.} \frac{1}{\mathbb{E}[\hat{f}(X, Y)]} \quad (21)$$

$$\frac{1}{N} \sum_{i=1}^N g(X_i, Y_i) \hat{f}(X_i, Y_i) \xrightarrow{a.s.} \mathbb{E}[g(X, Y) \hat{f}(X, Y)] \quad (22)$$

Assuming $\mathbb{E}[\hat{f}(X, Y)] \neq 0$, it follows that:

$$\hat{\beta}(x) \xrightarrow{a.s.} \min_{\beta(x)} \frac{\mathbb{E}[g(X, Y) \hat{f}(X, Y)]}{\mathbb{E}[\hat{f}(X, Y)]} \quad (23)$$

If $g(X, Y)$ and $\hat{f}(X, Y)$ are uncorrelated, then:

$$\mathbb{E}[g(X, Y) \hat{f}(X, Y)] = \mathbb{E}[g(X, Y)] \mathbb{E}[\hat{f}(X, Y)] \quad (24)$$

$$\hat{\beta}(x) \xrightarrow{a.s.} \min_{\beta(x)} \mathbb{E}[g(X, Y)] \quad (25)$$

Therefore, as $N \rightarrow \infty$:

$$\hat{\beta}(x) \xrightarrow{a.s.} \min_{\beta(x)} \mathbb{E} \left[\left(Y - \sum_{j=0}^p \beta_j(x)(x - X)^j \right)^2 K_{H_1}(x - X) \right] \quad (26)$$

¹⁵⁴ This is the same objective minimized by the standard LPR estimator in the asymptotic sense.
¹⁵⁵ Thus, the proposed estimator degenerates to the standard LPR as $N \rightarrow \infty$, provided that $g(X, Y)$
¹⁵⁶ and $\hat{f}(X, Y)$ are uncorrelated.

157 **5. Experiments and implementation notes**

158 The proposed method was implemented in Python. The distances between pairs are normalized
159 to the range [0,1] in each neighborhood as in [3]. The simple Laplacian kernel $e^{-\|x-x'\|}$ is
160 used for $K_1(x, x'; H_1)$ since it gave better and more efficient empirical results in tests than the
161 tricube kernel recommended in [3]. A factorized multidimensional KDE using scaled Gaussian
162 kernels is used for estimating the density. Five methods for estimating the bandwidth were used:
163 Scott's rule [12], Normal Reference, global LSCV, local LSCV and local MLCV. Additionally
164 the bandwidth for the predictor's kernel also uses in some of the experiments a simple function of
165 the window size estimated empirically. Certain computations are omitted for efficiency since the
166 local regression in equation (5) is invariant to the scale of the weights. This includes all scaling
167 constants fixed in a given neighborhood concerning a specific local regression target including
168 the computation of $\hat{f}(y|x)$ and $\hat{f}(x,y)$ in equations (7) and (11) respectively. Experiments were
169 performed on a number of synthetic benchmarks to evaluate the effectiveness of the method's
170 linear and quadratic variants in comparison to other methods of the local polynomial regression
171 family including LOWESS and iterative robust LOWESS [13], local linear and local constant
172 kernel regression [13], local quadratic regression [14] and radial basis function network [14].
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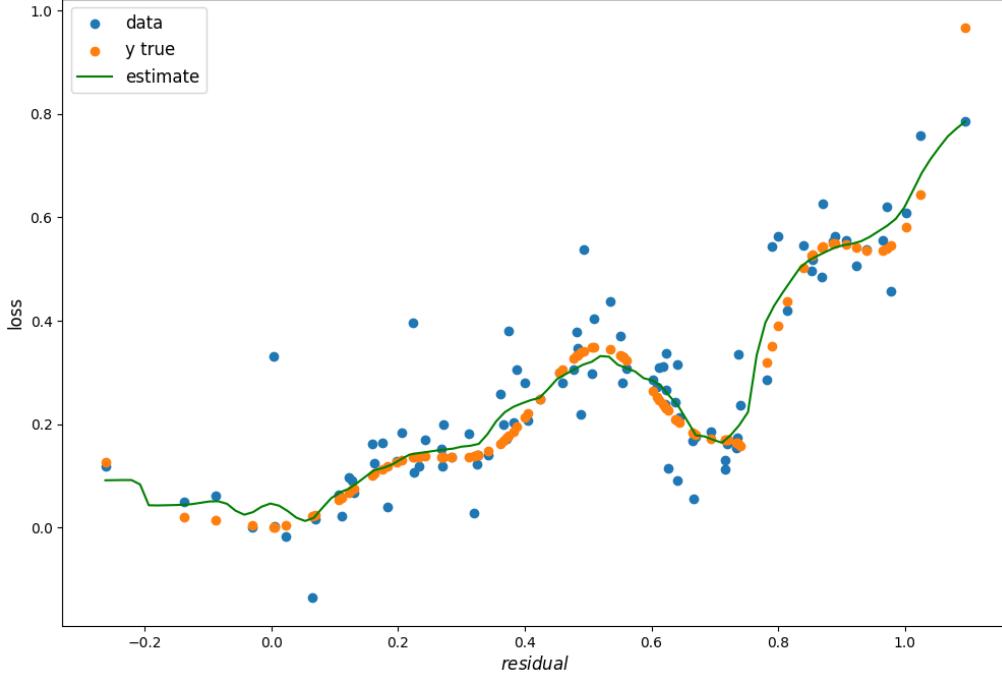
174 The experiments comprise a number settings including various non-linear synthetic curves
175 and planes with added noise. These have variants of dense and sparse data, homoscedastic and
176 heteroscedastic noise characteristics and various neighborhood sizes. The results indicate there
177 is no best universal method and that different methods work better in a given setting. However,
178 the proposed method offers competitive performance across the board and gives the best results
179 in a large number of settings and in particular in heteroscedastic settings. It is further shown the
180 proposed method generally improves on it's direct counterparts LOESS/LOWESS and quadratic
181 LPR using a single iteration. In addition it appears far less sensitive to the choice of neigh-
182 borhood size and has substantial reduced variance in this respect. This last quality makes it an
183 attractive choice since it is more likely for the analyst to select an "appropriate" hyperparameter
184 value when there is no ground truth available.

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186 The experimental results are available at <https://nbviewer.org/github/yaniv-shulman/rsklpr/tree/main/src/experiments/> as interactive Jupyter notebooks [1].
187

188 **6. Future work and research directions**

189 This work proposes a new robust variant of LPR and as such there are many aspects that need
190 to be explored and are left for future work. As the proposed method generalize the standard LPR
191 it does not preclude replacing some of the standard LPR components in equation (5) with other
192 and robust alternatives including robust methods for bandwidth selection and robust alternatives
193 to the standard quadratic residual function. Another avenue for developing this framework is
194 investigating additional kernels K_D and exploring the impact of robust density estimators on
195 performance.

Figure 3: Regression example of synthetically generated 1D data with heteroscedastic noise. Additional experimental results and demonstrations including multivariate settings and bootstrap based confidence intervals are available at <https://nbviewer.org/github/yaniv-shulman/rsklpr/tree/main/src/experiments/> as interactive Jupyter notebooks [1]



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196 References

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