# **Assignment 3**

CS215: Data Analysis and Interpretation

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# **Solutions**

#### **SOLUTION 1**

## Finding optimal bandwidth

#### Part 1

(a)

We are tasked with proving the following equation for the histogram estimator:

$$\int \hat{f}(x)^2 dx = \frac{1}{n^2 h} \sum_{j=1}^m v_j^2$$
 (1.1)

where  $\hat{f}(x)$  is the histogram estimator,  $v_j$  is the number of points in the j-th bin, n is the total number of points, h is the bin width, and m is the total number of bins.

The histogram estimator  $\hat{f}(x)$  is given by:

$$\hat{f}(x) = \sum_{j=1}^{m} \frac{\hat{p}_j}{h} \mathbb{1}_{[x \in B_j]}$$
 (1.2)

where  $\hat{p}_j = \frac{v_j}{n}$  is the estimated probability that a point falls in the *j*-th bin, and  $I_{[x \in B_j]}$  is the indicator function, which is 1 if  $x \in B_j$ , and 0 otherwise.

Now, square  $\hat{f}(x)$ :

$$\hat{f}(x)^2 = \left(\sum_{j=1}^m \frac{\hat{p}_j}{h} \mathbb{1}_{[x \in B_j]}\right)^2 \tag{1.3}$$

Since the bins  $B_i$  are non-overlapping, the cross terms vanish, and we are left with:

$$\hat{f}(x)^2 = \sum_{j=1}^m \left(\frac{\hat{p}_j}{h}\right)^2 \mathbb{1}_{[x \in B_j]}$$
(1.4)

Integrating  $\hat{f}(x)^2$  over the entire domain:

$$\int \hat{f}(x)^2 dx = \int \sum_{j=1}^m \left(\frac{\hat{p}_j}{h}\right)^2 \mathbb{1}_{[x \in B_j]} dx$$
 (1.5)

Because the bins  $B_i$  are disjoint, the integral breaks down into a sum of integrals over each bin:

$$\int \hat{f}(x)^2 dx = \sum_{j=1}^m \int_{B_j} \left(\frac{\hat{p}_j}{h}\right)^2 dx$$
 (1.6)

The length of each bin is h and  $\hat{p}_i/h$  is independent of x, so the integral over each bin  $B_i$  is:

$$\int_{B_j} 1 \, dx = h \tag{1.7}$$

Thus, we get:

$$\int \hat{f}(x)^2 dx = \sum_{j=1}^m \left(\frac{\hat{p}_j}{h}\right)^2 h = \frac{1}{h} \sum_{j=1}^m \hat{p}_j^2$$
 (1.8)

Recall that  $\hat{p}_j = \frac{v_j}{n}$ , so we can substitute  $\hat{p}_j^2$  as:

$$\hat{p}_{j}^{2} = \left(\frac{v_{j}}{n}\right)^{2} = \frac{v_{j}^{2}}{n^{2}} \tag{1.9}$$

Thus, the integral becomes:

$$\int \hat{f}(x)^2 dx = \frac{1}{h} \sum_{j=1}^m \frac{v_j^2}{n^2}$$
 (1.10)

Factor out  $\frac{1}{n^2h}$ :

$$\int \hat{f}(x)^2 dx = \frac{1}{n^2 h} \sum_{i=1}^m v_i^2$$
 (1.11)

Hence, proved.

#### (b)

Since  $\hat{f}_{(-i)}$  is defined as the histogram estimator after removing  $i^{\mathrm{th}}$  observation. We have

$$\hat{f}_{(-i)}(X_i) = \sum_{j=1}^m \frac{v_j - 1}{h(n-1)} \mathbb{1}_{[x \in B_j]}$$
(1.12)

Since the probability of  $x \in B_j$  is  $\frac{v_j}{n}$ 

$$\hat{f}_{(-i)}(X_i) = \sum_{j=1}^m \frac{v_j}{n} \frac{v_j - 1}{h(n-1)}$$
(1.13)

$$\sum_{i=1}^{n} \hat{f}_{(-i)}(X_i) = \sum_{i=1}^{n} \sum_{j=1}^{m} \frac{v_j}{n} \frac{v_j - 1}{h(n-1)}$$
(1.14)

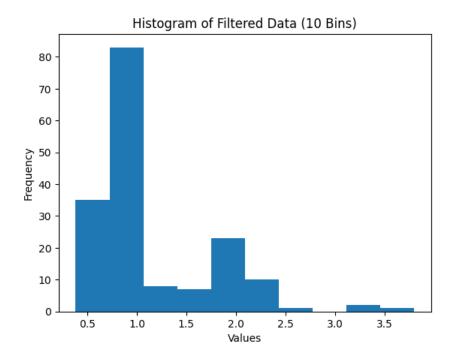
$$= \frac{1}{(n-1)h} \sum_{i=1}^{m} (v_j^2 - v_j)$$
 (1.15)

Hence Proved.

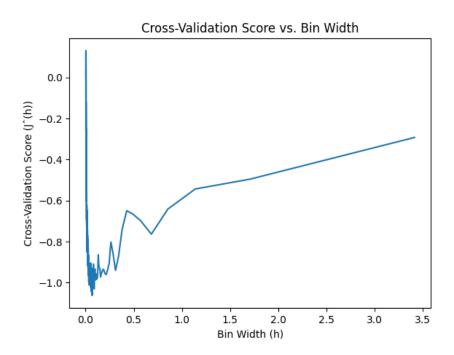
#### Part 2

(a) The estimated probabilities for all bins  $\hat{p}_j$  is given as:

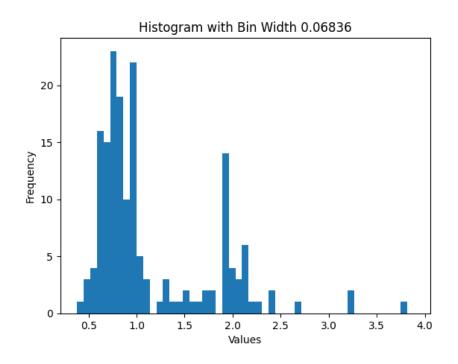
$p_1 = 0.2059$	$p_2 = 0.4882$
$p_3 = 0.0471$	$p_4 = 0.0412$
$p_5 = 0.1353$	$p_6 = 0.0588$
$p_7 = 0.0059$	$p_8 = 0.0000$
$p_9 = 0.0118$	$p_{10} = 0.0059$



- (b) The probability distribution is underfit. The binwidth is very large due to which the depiction of data is not quite smooth.
- (c) Here's the cross-validation plot:



- (d) The optimal binwidth h is 0.06836.
- (e) The plot seems to give a better analysis of the distribution. It offers significantly more detail and resolution compared to the 10-bin histogram. Each bin covers a narrower range of data values, leading to a more refined visualization that can better capture small variations in the dataset



SOLUTION 2

Detecting Anomalous Transactions using KDE

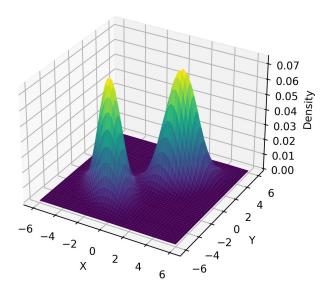


Figure 1.1: Distribution of transactions As can be seen in the given figure, the resulting estimated distribution contains two modes.

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#### **SOLUTION 3**

### **Higher-Order Regression**

#### Part 1

Suppose our estimates for  $\alpha$  and  $\beta$  are A and B respectively, then these values of A and B minimize

$$\sum_{i=1}^{n} (y_i - A - Bx_i)^2 \tag{1.1}$$

$$\implies \frac{\partial}{\partial A} \sum_{i=1}^{n} (y_i - A - Bx_i)^2 = 0 \tag{1.2}$$

$$\sum_{i=1}^{n} -2(y_i - A - Bx_i) = 0 \tag{1.3}$$

$$n\bar{y} - nA - nB\bar{x} = 0 \tag{1.4}$$

$$\bar{y} = A + B\bar{x} \tag{1.5}$$

Least square regression line is given by y = A + Bx. Thus by (1.5),  $(\bar{x}, \bar{y})$  lies on the regression line.

#### Part 2

Suppose our estimates for  $\beta_0^*$  and  $\beta_1^*$  are  $A^*$  and  $B^*$  respectively, then  $A^*$  and  $B^*$  minimize  $\sum_{i=1}^n (y_i - A^* - B^*z_i)^2$ 

$$\implies \frac{\partial}{\partial A^*} \sum_{i=1}^n (y_i - A^* - B^* z_i)^2 = 0 \qquad \qquad \frac{\partial}{\partial B^*} \sum_{i=1}^n (y_i - A^* - B^* z_i)^2 = 0$$
 (1.6)

$$\sum_{i=1}^{n} -2(y_i - A^* - B^* z_i) = 0 \qquad \qquad \sum_{i=1}^{n} -2z_i (y_i - A^* - B^* z_i) = 0$$
 (1.7)

$$n\bar{y} - nA^* - nB^*\bar{z} = 0$$
 
$$\sum z_i y_i - A^* n\bar{z} - B^* \sum z_i^2 = 0$$
 (1.8)

$$\sum y_i z_i - n(\bar{y} - B^* \bar{z}) \bar{z} - B^* \sum z_i^2 = 0$$
 (1.9)

$$B^* = \frac{\sum y_i z_i - n\bar{y}\bar{z}}{n\bar{z}^2 - \sum z_i^2}$$
  $A^* = \bar{y} - B^*\bar{z}$  (1.10)

Since,  $z_i = x_i - \bar{x}$ .  $\bar{z} = \frac{\sum (x_i - \bar{x})}{n} = \frac{n\bar{x} - n\bar{x}}{n} = 0$ .  $\sum (x_i - \bar{x})^2 = \sum x_i^2 - n\bar{x}^2$ 

$$B^* = \frac{\sum y_i(x_i - \bar{x}) - n\bar{y} \cdot 0}{n(0)^2 - (\sum x_i^2 - n\bar{x}^2)}$$
(1.11)

$$=\frac{\sum y_i x_i - n\bar{x}\bar{y}}{n\bar{x}^2 - \sum x_i^2} \tag{1.12}$$

This is same as B, least square estimate of  $\beta_1$  i.e  $B^*=B$ . Also since  $\bar{z}=0$ , we have  $A^*=\bar{y}$  i.e  $A^*=A+B\bar{x}$ , where A is the least square estimate of  $\beta_0$ .

#### Part 3

Let's restrict ourselves to single feature for simplicity. Suppose we have n data points

$$\{(x_1, y_1), \dots, (x_n, y_n)\}\$$
 (1.13)

and our OLS estimates for  $\beta_0, \ldots, \beta_m$  be  $B_0, \ldots, B_m$ . These must minimize

$$\sum_{i=1}^{n} (y_i - B_0 - B_1 x_i - \dots - B_m x_i^m)^2$$
 (1.14)

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Partial differentiation w.r.t each  $B_i$  must be 0 which gives

$$\sum_{i=1}^{n} -2(y_i - B_0 - B_1 x_i - \dots - B_m x_i^m) = 0$$
 (1.15)

$$\sum_{i=1}^{n} -2x_i(y_i - B_0 - B_1x_i - \dots - B_mx_i^m) = 0$$
(1.16)

 $\vdots \qquad (1.17)$ 

$$\sum_{i=1}^{n} -2x_i^m (y_i - B_0 - B_1 x_i - \dots - B_m x_i^m) = 0$$
(1.18)

Which give

$$\sum_{i=1}^{n} y_i = B_0 n + B_1 \sum_{i=1}^{n} x_i + \dots + B_m \sum_{i=1}^{n} x_i^m$$
(1.19)

$$\sum_{i=1}^{n} x_i y_i = B_0 \sum_{i=1}^{n} x_i + B_1 \sum_{i=1}^{n} x_i^2 + \dots + B_m \sum_{i=1}^{n} x_i^{m+1}$$
(1.20)

$$\sum_{i=1}^{n} x_i^m y_i = \sum_{i=1}^{n} B_0 x_i^m + B_1 \sum_{i=1}^{n} x_i^{m+1} + \dots + B_m \sum_{i=1}^{n} x_i^{2m}$$
(1.22)

Taking 
$$X = \begin{bmatrix} 1 & x_1 & \dots & x_1^m \\ 1 & x_2 & \dots & x_2^m \\ \vdots & \vdots & \ddots & \vdots \\ 1 & x_n & \dots & x_n^m \end{bmatrix}$$
,  $Y = \begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix}$ ,  $B = \begin{bmatrix} B_0 \\ \vdots \\ B_m \end{bmatrix}$  we have

$$X^TY = X^TXB (1.23)$$

$$B = (X^T X)^{-1} X^T Y (1.24)$$

We'll use this in our code.

#### **Conclusions**

- 1. By the SSR graph above, m=18 seems to be the optimal degree of the polynomial. Thus, polynomial regressor of degree 18 would be the best fit regressor for this data.
- 2.  $SS_R$ 's values are too close so values close aren't too much of an underfit/overfit (they're almost similar) We see that  $SS_R$  at 2 and 21 have comparatively high  $SS_R$ s, so degree 2 can be considered as an underfit and degree 21 as an overfit. Here's the fit for underfit, optimal fit and overfit respectively
- 3. At the end these are the values obtained:
  - $SS_R = 224592.60834798065$
  - $R^2 = 0.910251432520619$

#### **SOLUTION 4**

### Non-parametric regression

#### Report Bandwidth Corresponding to Minimum Estimated Risk

After running the Nadaraya-Watson kernel regression using the Epanechnikov and Gaussian kernel and performing cross-validation for bandwidth selection, the optimal bandwidth corresponding to the minimum estimated risk is:

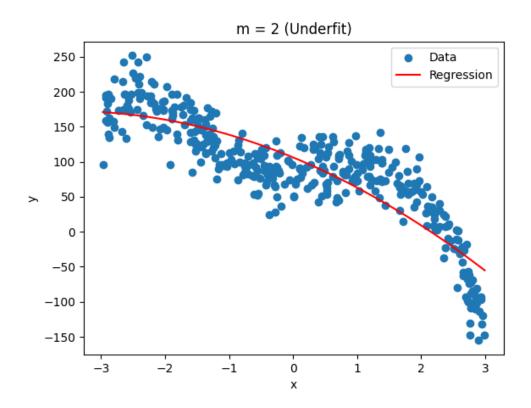


Figure 1.2: Underfit model

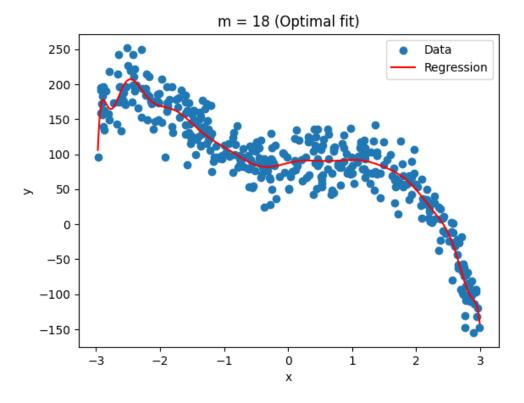


Figure 1.3: Optimal model

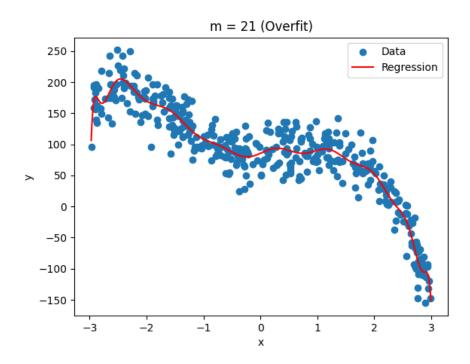


Figure 1.4: Overfit model

- Optimal Bandwidth of Gaussian kernel: 0.180
- Optimal Bandwidth of Epanechnikov kernel: 0.164

# Similarities and Differences Due to Choice of Different Kernel Functions Similarities

- **General Functionality:** Both kernels assign weights to data points based on their distance from the query point, resulting in similar predictions in regions with high data density.
- Smoothing: As the bandwidth increases, all kernel functions produce smoother estimates. At very large bandwidths, all kernels oversmooth the data, giving too much influence to distant points.
- Cross-validation Behavior: Both kernels display a similar behavior during cross-validation, and the corresponding risk curves follow the same trend with bandwidth changes.

#### Differences

- Shape of the Weights:
  - Epanechnikov Kernel: This kernel assigns zero weight to points farther than the bandwidth due to its quadratic form, creating a more localized effect.
  - Gaussian Kernel: This kernel assigns non-zero weight to every point, regardless of distance, due to its exponential decay. It results in smoother estimates, but it is more sensitive to distant points.
- Sensitivity to Outliers:
  - **Epanechnikov Kernel:** This kernel is more resilient to outliers because they assign zero or reduced weight to distant points, decreasing the influence of outliers on the prediction.

- **Gaussian Kernel:** The Gaussian kernel is more prone to incorporating outliers, as it assigns non-zero weights even to far-away points, making it less resilient in the presence of outliers.

#### • Plots

- **Epanechnikov Kernel:** This kernel produces more precise and localized estimates, with a good balance between bias and variance when using the optimal bandwidth.
- Gaussian Kernel: The Gaussian kernel leads to smoother curves but gives undue influence to distant points, which can result in overfitting or oversmoothing depending on the bandwidth.

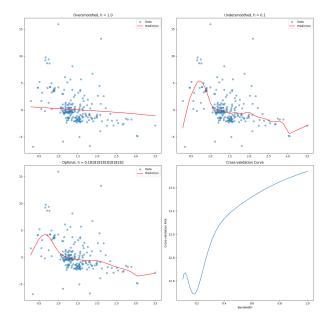


Figure 1.5: Oversmoothed, undersmoothed, optimal and cross validation curve of gaussian kernel

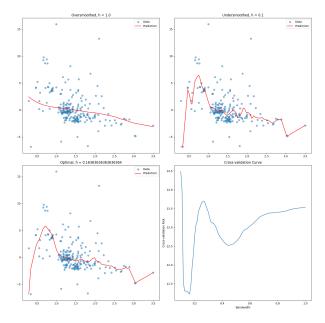


Figure 1.6: Oversmoothed, undersmoothed, optimal and cross validation curve of epanechnikov kernel