### Problem Set: Non Parametric Statistics: Group 18

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#### Question 1

#### Question 2

Compare the MISE and AMISE criteria in three densities in nor1mix of your choice.

- 1. Code (2.33) and the AMISE expression for the normal kernel, and compare the two error curves.
- 2. Compare them for n = 100, 200, 500, adding a vertical line to represent the  $h_{MISE}$  and  $h_{AMISE}$  bandwidths. Describe in detail the results and the major takeaways.

For this exercise we require some mathematical ideas that we will developed briefly.

We start with the KDE estimator  $\hat{f}(x;h) = \sum_{i=1}^{n} K_h(x-X_i)$ . The expectation and variance for this estimator are given bit he following expressions:

(1) 
$$E[\hat{f}(x;h)] = (K_h * f)(x)$$
.

(2) 
$$\operatorname{Var}[\hat{f}(x;h)] = \frac{1}{n}((K_h^2 * f)(x) - (K_h * f)^2(x))$$

Then, we develop some assymptotic expression for (1) and (2):

(3) 
$$E[\hat{f}(x;h)] - f(x) = Bias[\hat{f}(x;h)] = \frac{1}{2}\mu_2(K)f''(x)h^2 + o(h^2)$$

(4) 
$$\operatorname{Var}[\hat{f}(x;h)] = \frac{R(K)}{nh} f(x) + o((nh)^{-1})$$

Then, from whe equations (3) and (4) we obtain the following expression for the MSE:

(5) 
$$MSE[\hat{f}(x;h)] = \frac{\mu_2^2(K)}{4} (f''(x))^2 h^4 + \frac{R(K)}{nh} f(x) + o(h^4 + (nh)^{-1})$$

In equations (3), (4) and (5) we have:

(6) 
$$\mu_2(K) := \int z^2 K(z) dz$$

(7) 
$$R(K) := \int (K(x))^2 dx$$

Then, we use  $\text{MISE}[\hat{f}(\cdot;h)]$  as global error criteria for measuring the performance of  $\hat{f}$  in relation to the target density f.

(8) 
$$MISE[\hat{f}(\cdot;h)] = \int MSE[\hat{f}(x;h)]$$

Then, we obtain the following asymptotic expansion for the MISE:

(9) 
$$\text{MISE}[\hat{f}(\cdot;h)] = \frac{1}{4}\mu_2^2(K)R(f^{"})h^4 + \frac{R(K)}{nh} + o(h^4 + (nh)^{-1})$$

We define the dominating part of equation (9) as  $AMISE[\hat{f}(\cdot;h)]$  defined as:

(10) AMISE
$$[\hat{f}(\cdot;h)] = \frac{1}{4}\mu_2^2(K)R(f'')h^4 + \frac{R(K)}{nh}$$

with the expression R(f'') given by:

(11) 
$$R(f'') = \int (f''(x))^2 dx$$

Finally, the bandwidth the minimizes the AMISE is:

(12) 
$$h_{AMISE} = \left[ \frac{R(K)}{\mu_2^2(K)R(f'')n} \right]^{1/5}$$

Now, we consider our particular case of study. In this case, we reduce our analysis considering:

- a) A normal kernel  $K_h(\cdot)$  with distribution  $\mathcal{N}(0,1)$
- b) The density function f is based on the family of normal r-mixtures:

(13) 
$$f(x; \mu, \sigma, \mathbf{w}) = \sum_{j=1}^{r} w_j \phi_{\sigma_j}(x - \mu_j)$$

where 
$$w_j \ge 0, j = 1, ..., r$$
 and  $\sum_{j=1}^{r} w_j = 1$ .

With this two expression, we can obtain a specific value for the AMISE in equation (10). With assumption a), we obtain the following expressions for equations (6) and (7)

(6.1) 
$$\mu_2(K) = 1$$

(7.1) 
$$R(K) = \frac{1}{2\sqrt{\pi}}$$

Expression for equation (11) can be obtained from the following adaption of expression given in *Theorem 4.1* given by *Marron and Wand (1992)* 

(11.1) 
$$R(f'') = \int (f''(x))^2 dx =$$

With this expression, we obtain the reduced form of the AMISE:

(10.1) AMISE
$$[\hat{f}(\cdot;h)] = \frac{1}{4}R(f'')h^4 + \frac{1}{2nh\sqrt{\pi}}$$

With optimal bandwidth  $h_{AMISE}$ 

(12.1) 
$$h_{AMISE} = \left[ \frac{(2\sqrt{\pi})^{-1}}{R(f'')n} \right]^{1/5}$$

Finally, under this assumptions, we obtain a explicit and exact MISE expression of equation (8):

(14) 
$$\mathrm{MISE}_{r}[\hat{f}(\cdot;h)] = (2\sqrt{\pi}nh)^{-1} + \boldsymbol{w}'\{(1-n^{-1})\Omega_{2} - \Omega_{1} + \Omega_{0}\}\boldsymbol{w}$$

with 
$$(\Omega_a)_{i,j} = \phi_{(ah^2 + \sigma_i^2 + \sigma_i^2)^{1/2}}(\mu_i - \mu_j)$$
 for  $i, j = 1, ..., r$ 

Finally, we can proceed with a numeric approach over equation (14) and obtain:

(15) 
$$\arg \min_{h>0} \mathrm{MISE}[\hat{f}(\cdot;h)]$$

We start with a easy example using the dataset nor1mix::MW.nm1 that is distributed according to  $\mathcal{N}(0,1)$ 

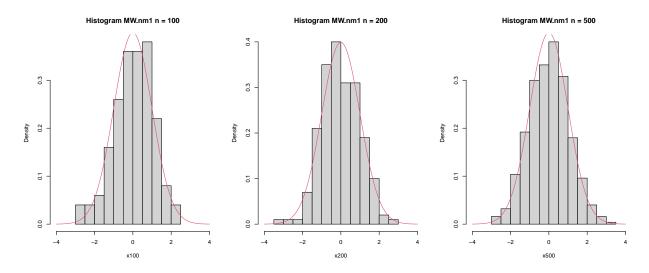


Figure 1: Histograms from sample obtained from n = 100, 200 and 500 for object MW.nm1

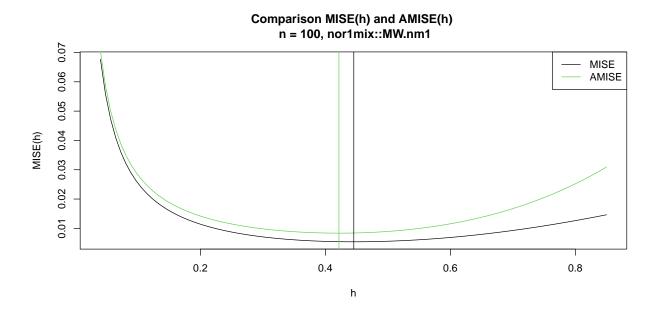


Figure 2: MISE and AMISE for range bandwith between 0.04 and 0.85 and n=100

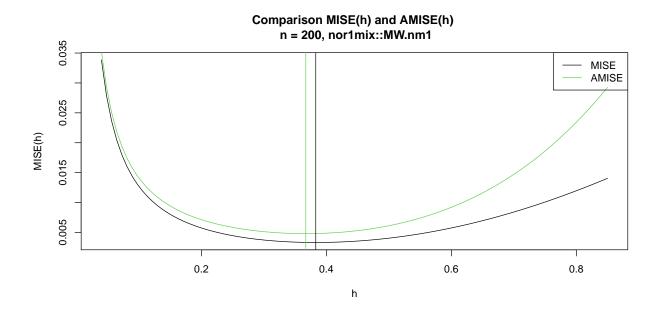


Figure 3: MISE and AMISE for range bandwith between 0.04 and 0.85 and  $\rm n=200$ 

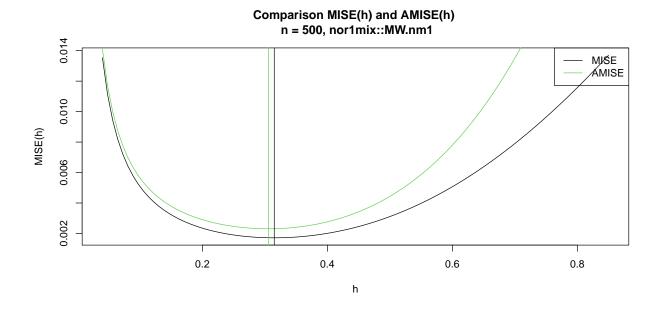


Figure 4: MISE and AMISE for range bandwith between 0.04 and 0.85 and n=500

#### Question 3

Adapt the np\_pred\_CI function to include the argument type\_boot, which can take either the value "naive" or "wild".

- 1) If type\_boot = "wild", then the function must perform the wild bootstrap algorithm, implemented from scratch following substeps i-iv.
- 2) Compare and validate the correct behavior of the confidence intervals, for the two specifications of type\_boot, in the model considered in Exercise 5.8 (without performing the full simulation study).

For this question we describe briefly the necessary steps related to the implementation of the wild-bootstrap:

First of all, for a given sample with n observations, the predicted (fitted) values are given by the expression:  $\hat{Y}_i := \hat{m}(X_i; q, h)$  with i = 1, ..., n.

Then, the uncertainty of  $\hat{m}(x, q, h)$  (this includes the consideration of new set of samples) can be measure based on two approaches:

- 1. Asymptotic approach:  $\hat{m}(x;q,h) \pm \hat{se}(\hat{m}(x;q,h))$  where  $\hat{se}(\hat{m}(x;q,h))$  is the asymptotic estimation of the standard deviation of  $\hat{m}(x;q,h)$
- 2. Bootstrap: In this case, we consider two types of bootstrap:
- $\bullet\,$  Naive Bootstrap: From the original sample, we create a new set of IID observations called the Bootstrap sample
- Wild Bootstrap: This technique is focused on resampling the residuals. Similar to the residual bootstrap in which we fixed the covariate  $X_i$  and generate a new value of  $Y_i$  using the fitted model and the noise from sampling the residuals, additional we generate IID random variables  $V_i$  (random variable with mean zero and variance 1) and then we can perturb the residuals. This modification improves the stability of the computations, especially in the presence of heteroskedasticity.

The algorithm of the computation of the wild boostrap is given in the following steps:

- 1. Compute  $\hat{m}(x;q,h) = \sum_{i=1}^{n} W_i^q(x) Y_i$  from the original sample  $(X_1,Y_1),...,(X_n,Y_n)$
- 2. Enter the wild bootstrap. For b = 1, ..., B.
- i. Simulate  $V_1^{*b}, ..., V_n^{*b}$  to be iid copies of V such that E[V] = 0 and Var[V] = 1,
- ii. Compute the pertubed residuals  $e_i^{*b} = \hat{e}_i V_i^{*b}$  where  $Y_i^{*b} := \hat{m}(X_i; q, h) + e_i^{*b}$  for i = 1, ..., n.
- iii. Obtain the bootstrap sample:  $(X_1, Y_1^{*b}), ..., (X_n, Y_n^{*b})$  where  $Y_i^{*b} := \hat{m}(X_i; q, h) + e_i^{*b}$  with i = 1, ..., n.
- iv. Compute  $\hat{m}^{*b}(x;q,h) = \sum_{i=1}^n W_i^q(x) Y_i^{*b}$  from  $(X_1^*,Y_1^{*b}),...,(X_n^8,Y_n^{*b})$

As a result, we modified the function np\_pred\_CI. The inputs of the original function are the following:

- 1. npfit: A np::npreg object (npfit)
- 2. exdat: Values of the predictors were to carry out prediction (exdat)
- 3. B: Number of bootstrap iterations.

4.conf: Range of confidence interval

5. type\_CI: Type of confidence interval. (Normal standard or quantiles)

Additionally, we add three new inputs:

- 6. type\_boot: Type of bootstrap procedure. Options: Naive and Wild bootstrap
- 7. perturbed\_res: For the case of Wild Bootstrap, we can choose the type of perturbation. As explained before, any random variable with mean 0 and variance 1 can be used. As a result, we use two possible perturbation:

- 7.1. normal: Based on the normal distribution  $V_i \sim \mathcal{N}(0,1)$
- 7.2 golden: Based on the golden section binary variable  $P[V=1-\phi]=p, P[V=\phi]=1-p$  and  $p=\frac{\phi+2}{5}$ 
  - 8. seed: Used for reproducibility. Default option is seed = 42.

The code of the new version of np\_pred\_CI is given below. We create a new if condition, in order to compute the type of bootstrap resampling method chosen by the user. In the case of the wild bootstrap, we focus on resampling the residuals obtained from the difference of the fitted value  $\hat{Y}_i$  and the real values  $Y_i$ . Moreover, inside the option type\_boot == wild, there is an if condition with the two possible alternatives for computing the perturbed residuals.

```
# Function to predict and compute confidence intervals for m(x).
# 1) Inputs
## 1.1) npfit: A np::npreq object (npfit)
## 1.2) exdat: Values of the predictors where to carry out prediction (exdat)
               Number of bootstrap iterations.
## 1.3) B:
## 1.4) conf: Range of confidence interval
## 1.5) type_CI: Type of confidence interval. (Based on normal standard or quantiles)
## 1.6) type_boot: Type of bootstrap procedure. Options Naive and Wild bootstrap
## 1.7) perturbed_res: Valid only for Wild Bootstrap. Type of perturbation on the residuals.
## Options are "normal"or "golden"
## 1.8) seed: Used for reproducibility. Default option is seed = 42.
# 2) Outputs
## 2.1) exdat: Values of the predictors where to carry out prediction
## 2.2) m_hat: Predicted regression
## 2.3) lwr: Lower confidence interval
## 2.4) upr: Upper confidence interval
np_pred_CI <- function(npfit,</pre>
                        exdat,
                        B = 200.
                        conf = 0.95,
                        type_CI = c("standard", "quantiles")[1],
                        type_boot = c("naive", "wild")[1],
                        perturbed_res = c("normal", "golden")[1],
                        seed = 42) {
  # Fix seed
  set.seed(seed)
  # Extract predictors
  xdat <- npfit$eval</pre>
  \# Extract response, using a trick from np::npplot.rbandwidth
  tt <- terms(npfit$bws)</pre>
  tmf <- npfit$bws$call[c(1, match(c("formula", "data"),</pre>
                                    names(npfit$bws$call)))]
  tmf[[1]] <- as.name("model.frame")</pre>
  tmf[["formula"]] <- tt</pre>
  tmf <- eval(tmf, envir = environment(tt))</pre>
  ydat <- model.response(tmf)</pre>
```

```
\# Predictions m_hat from the original sample
m_hat <- np::npreg(txdat = xdat,</pre>
                    tydat = ydat,
                    exdat = exdat,
                    bws = npfit$bws)$mean
if (type_boot == "naive") {
  # Function for performing naive bootstrap
 boot_function_naive <- function(data, indices) {</pre>
    np::npreg(txdat = xdat[indices,],
              tydat = ydat[indices],
              exdat = exdat,
              bws = npfit$bws)$mean
 }
  # Carry out the bootstrap estimator
 m_hat_star <- boot::boot(data = data.frame(xdat),</pre>
                            statistic = boot_function_naive,
                            R = B)$t
} else if (type_boot == "wild") {
  # Sample size of the predictors
 n <- length(xdat)</pre>
  # Y fitted
 Y_hat <- npfit$mean
  # Ordinary residuals
 residuals_0 <- Y_hat - ydat
  # Type of perturbation
  if(perturbed_res == "normal"){
    # Function for performing wild bootstrap
    boot_function_wild <- function(data, indices) {</pre>
      \# Step i: Simulate V_{i} copies of V (Mean 0 and variance 1)
      V n <- rnorm(n)</pre>
      # Step iii. Obtain the bootstrap sample
      ydat_bt <- Y_hat + data[indices]*V_n</pre>
      np::npreg(txdat = xdat,
                tydat = ydat_bt,
                exdat = exdat,
                bws = npfit$bws)$mean
    }
    # Step iv. Carry out the wild bootstrap estimator
    m_hat_star <- boot::boot(data = residuals_0,</pre>
                              statistic = boot_function_wild,
```

```
R = B)$t
  } else if(perturbed_res == "golden"){
    # Function for performing wild bootstrap
    boot_function_wild <- function(data, indices) {</pre>
      # Step i: Simulate V_{i} copies of V (Mean 0 and variance 1)
      phi <- (1 + sqrt(5))/2
      prob <- (phi + 2)/5
      golden <- sample(x = c(1-phi,phi), size = n, prob = c(prob, 1 - prob), replace=T)</pre>
      # Step iii. Obtain the bootstrap sample
      ydat_bt <- Y_hat + data[indices]*golden</pre>
      np::npreg(txdat = xdat,
                tydat = ydat_bt,
                 exdat = exdat,
                 bws = npfit$bws)$mean
    }
    # Step iv. Carry out the wild bootstrap estimator
    m_hat_star <- boot::boot(data = residuals_0,</pre>
                              statistic = boot function wild,
                               R = B)$t
  }
  else{stop("Incorrect type of peturbation")}
}else{stop("Incorrect type_boot")}
# Confidence intervals
alpha \leftarrow 1 - conf
if (type_CI == "standard") {
  z \leftarrow qnorm(p = 1 - alpha / 2)
  se <- apply(m_hat_star, 2, sd)</pre>
  lwr \leftarrow m_hat - z * se
  upr <- m_hat + z * se
} else if (type_CI == "quantiles") {
  q <- apply(m_hat_star, 2, quantile, probs = c(alpha / 2, 1 - alpha / 2))
  lwr <- q[1, ]</pre>
  upr \leftarrow q[2,]
} else {
  stop("Incorrect type_CI")
# Return evaluation points, estimates, and confidence intervals
```

```
return(data.frame("exdat" = exdat, "m_hat" = m_hat, "lwr" = lwr, "upr" = upr))
}
```

Finally, we compare and validate the correct behavior of the confidence intervals, for the two specifications of type\_boot and the two types of perturbations. For this purpose, we simulate the following sample of size n = 100 from the regression model  $Y = m(x) + \epsilon$  where  $m(x) = 0.25x^2 - 0.75x + 3$ , with  $X \sim \mathcal{N}(0, 1.5^2)$  and  $\epsilon \sim (0, 0.75^2)$ . Figure 5 shows the simulated sample. In this case the simulated observations are concentrated in the left side of the plot.

#### Simulate observations m(x)

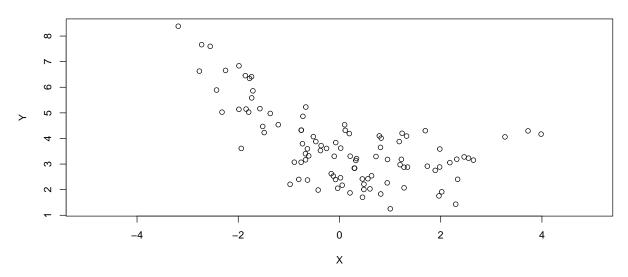


Figure 5: Simulation of 100 observations for m(X). Seed = 12345

Then, we fit a model using the function npregbw() with regtype = "lc" and the final model is created with the function npreg(). For reference, figures 6 and 7 shows the confidence interval under normal approximation and quantile compute by np::npplot. In particular, we focus on the right side of the confidence intervals. In the case of quantile confidence interval (figure 7) the upper confidence bound is relatively close to the fitted regression  $\hat{m}(X_i;q,h)$ 

# Bootstrap (npplot) Normal Approximation Confidence Intervals

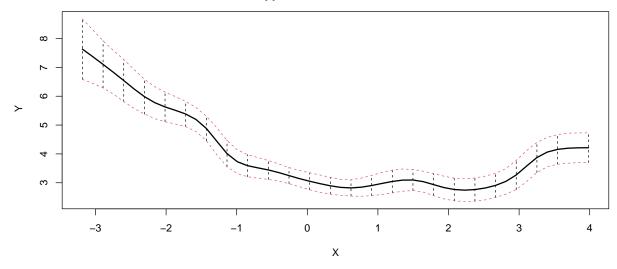
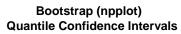


Figure 6: Bootstrap intervals: Default option npplot



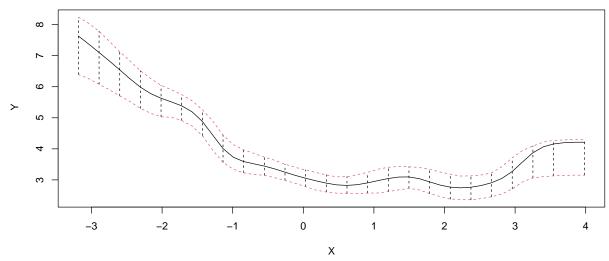


Figure 7: Bootstrap intervals: Default option npplot

Then, we compute 95% confidence intervals for m(x) along x <- seq(-5, 5, by = 0.1). Figure 8 shows the case of the naive bootstrap. In this case, we see how the confidence intervals of the default quantile option of np::npplot coincide perfectly with the confidence interval given by np\_pred\_CI with the option type\_bot = naive. Additionally, the light blue and green lines represents the extension of the predicted values for m(x) in the grid between -5 and 5.

### Confidence Intervals quantile Naive Bootstrap

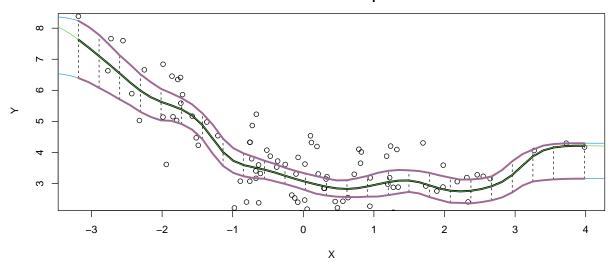


Figure 8: Function np\_pred\_CI: Naive Bootstrap

Finally, figures 9 and 10 shows the confidence intervals in case of wild bootstrap with normal and golden section perturbation. In this case, we notice how the confidence interval is in the function of the number of simulated observations. In the case of the tails, especially on the right side, the confidence intervals are wider in relation to the confidence intervals given by the naive bootstrap. On the other hand, in the sections of the graph where there is a concentration of simulated observations, the fitted lower and upper confidence intervals are similar for the two bootstrap methodologies.

## Confidence Intervals quantile Wild Bootstrap – Normal perturbation

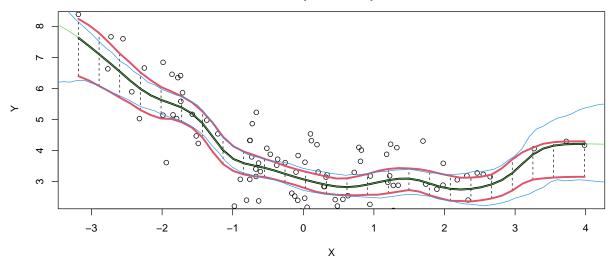


Figure 9: Function np\_pred\_CI: Wild Bootstrap and normal perturbation

## Confidence Intervals quantile Wild Bootstrap – Golden ratio perturbation

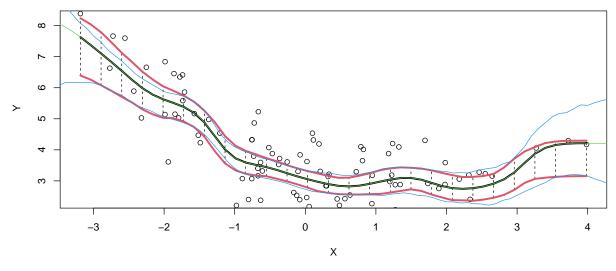


Figure 10: Function np\_pred\_CI: Wild Bootstrap and golden error perturbation