(EP-2): K-M Estimation, Kernel Regression and Spline

Yuan Gao, Kevin Lee, Akshay Govindaraj, Yijun (Emma) Wan, Peter Williams, Ruixuan Zhang

Date: 2018-11-16

Contents

Workload Distribution	2
Problems	3
1. K-M Estimation (25%):	3
2. Kernel and Related Regression with One Explanatory Variable (40%):	4
3. Cross-Validation With the "Leave-One-Out" Procedure (10%):	12
4. Resampling Procedures: Bootstrap and Jackknife (25%):	12
Code Appendix	12

Workload Distribution

Workload and description of tasks completed by each team member for this project:

Team Member	Task Description
Yuan Gao	TBD
Kevin Lee	Loess, Smoothing Splines, Part of Regression Comparison
Akshay Govindaraj	TBD
Yijun (Emma) Wan	TBD
Peter Williams	Code Compilation, Data Visualization & Latex Formatting
Ruixuan Zhang	TBD

Problems

1. K-M Estimation (25%):

Locate a data set with right-censoring (in Type-I Censoring) in the field of your interest, e.g., eCommerce, medical study, drug development, supply-chain/logistics operations, for applying the K-M Estimator to estimate the survival function with pointwise confidence intervals. Is it possible to locate a software program that can provide the confidence band for the K-M estimate?

For this exercise, we located a dataset, that consists of measures on, n = 69, different patients who received a heart transplant, taken from the first edition of the text *The Statistical Analysis* of Failure Time Data by Kalbfleisch and Prentice, Appendix I (230-232), published originally in 1980, which can also be found via the following link on the Carnegie Mellon statistics site: http://lib.stat.cmu.edu/datasets/stanford, and has three columns with the following measures:

- Age: Age of patient in years at the time of heart transplant in years
- Status: Survival status (1=dead, 0=alive)
- Days: Survival time in days after transplant (in days)

A preview of this dataset is provided here:

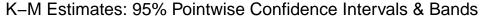
Table 1: Preview: Heart Transplant Data

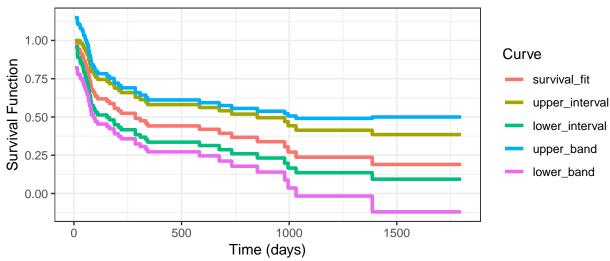
Age	Status	Days
41	1	5
40	1	16
35	0	39
50	1	53
45	1	68
26	0	180

This dataset is right censored, because as shown above, we don't exactly how long patients who currently have a (status=0) will survive, or survived.

Utilizing this dataset, and the *survival* package in R, we generate the Kaplan-Meier estimates, and visualize the survival function, i.e. $S_{KM}(x_{i:n}) = 1 - F_{KM}(x_{i:n})$, with confidence intervals below, visualized in the first plot below.

In the second plot, relying on the, the km.ci R package which can be found in the CRAN repository, in R which provides a number of confidence intervals and band for the Kaplan-Meier estimator. To compute confidence bands, the km.ci package has an option to utilize the estimation procedure detailed in $Confidence\ bands$ for a $survival\ curve\ from\ censored\ data$, authored by W.J. Hall, and Jon A. Wellner, in the journal Biometrika in 1980. Code to reproduce these plots is provided in the code appendix:





Visual analysis of the plot here, indicates that the probability of survival for 500 days, after a heart transplant is approximately 42%, with a 95% confidence range of approximately 30-55%, among patients in this data, when this data was collected decades ago. We hope that survival rates have improved since this study was conducted many years ago.

The plot also clearly show that the *Hall-Wellner* confidence bands are wider than corresponding pointwise confidence intervals across time.

2. Kernel and Related Regression with One Explanatory Variable (40%):

Locate a data set suitable for nonparametric regression (usually has nonlinear y-x relationship) in the field of your interest, e.g., eCommerce, medical study, drug development, supply-chain/logistics operations. Apply all of the procedures below:

- 1) Kernel Regression,
- 2) Local Polynomial Regression,
- 3) LOESS.
- 4) Smoothing Spline, to the y-x data-fit.
 - Compare fits from the four methods.

 For this exercise, we located another dataset, that consists of Data give the mortality rate and the education level for 58 U.S. cities. It can be found via the following link on the *The Data And Story Library* site:https://dasl.datadescription.com/datafile/education-and-mortality, and has two columns with the following measures:
- Mortality: the mortality rate (deaths per 100,000 people)
- Education: the average number of years in school
- 1) Kernel Regression,

```
rdat <- read.csv('data/education-and-mortality.csv',header=T,stringsAsFactors=F)
bw <- npregbw(formula=rdat$Mortality~rdat$Education, tol=.1, ftol=.1)</pre>
##
Multistart 1 of 1 |
# Now take these bandwidths and fit the model and gradients
model <- npreg(bws = bw, gradients = TRUE)</pre>
summary(model)
##
## Regression Data: 58 training points, in 1 variable(s)
##
                  rdat$Education
## Bandwidth(s):
                       0.4382052
##
## Kernel Regression Estimator: Local-Constant
## Bandwidth Type: Fixed
## Residual standard error: 47.22676
## R-squared: 0.4196534
##
## Continuous Kernel Type: Second-Order Gaussian
## No. Continuous Explanatory Vars.: 1
npplot(bws=bw, plot.errors.method="bootstrap",col = "blue")
points(rdat$Education, rdat$Mortality, cex=.2, col="red")
        1000
   rdat$Mortality
        950
        900
            9.5
                        10.0
                                    10.5
                                                11.0
                                                             11.5
                                                                         12.0
```

2) Local Polynomial Regression,

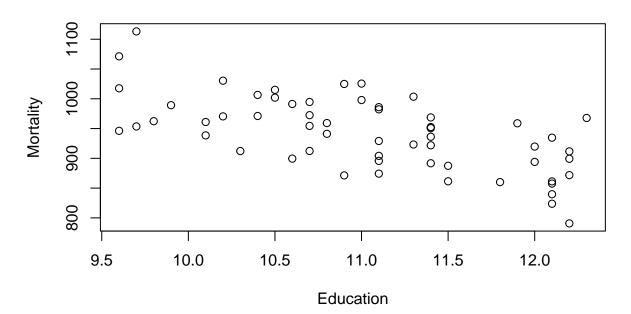
rdat\$Education

```
fit <- locfit(Mortality~lp(Education,deg=4),data=rdat)</pre>
summary(fit)
## Estimation type: Local Regression
##
## Call:
## locfit(formula = Mortality ~ lp(Education, deg = 4), data = rdat)
##
## Number of data points:
                            58
## Independent variables:
                            Education
## Evaluation structure: Rectangular Tree
## Number of evaluation points: 5
## Degree of fit: 4
## Fitted Degrees of Freedom: 6.982
crit(fit) <- crit(fit,cov=0.99)</pre>
plot(fit,band='local')
points(rdat$Education, rdat$Mortality, cex=.2, col="red")
        1050
  Mortality
        950
        850
            9.5
                        10.0
                                    10.5
                                                11.0
                                                            11.5
                                                                         12.0
                                            Education
res <- residuals(fit)</pre>
des <- rdat$Mortality-mean(rdat$Mortality)</pre>
r_{square} = 1 - sum((res)^2/sum((des)^2))
  3) LOESS,
#Making our variables easy to use in modeling
Mortality=rdat[,1]
Education=rdat[,2]
#packages to help create colors for plotting smoothing lines
library(RColorBrewer)
library(sp)
```

Loess models, with varying spans, with degree=1. When interpreting the summary results for the loess models, we will notice that increasing span will decrease the SSR but the curve of the model will become more jagged, making it so that the curve may not be the best representation. Loess is mostly a visual tool to see curves for non-linear curves through the use of data to form the line rather than a specified mathematical model. Loess is based purely on the span and degree of the polynomial (quadratic or linear) for the potential loess model. For the purposes of demonstrating this technique on our data, we will use loess models with a degree of "1" which indicates a linear smoothing function compared to a quadratic form. Below, different spans are utilized to show the effect the span value has on the appearance of the curve.

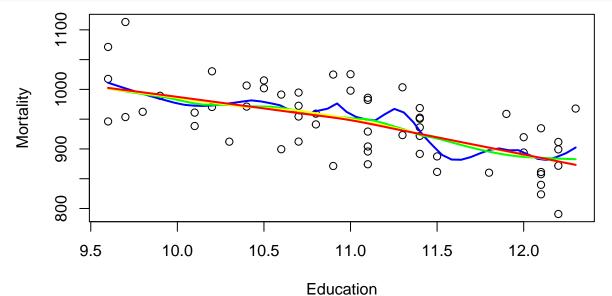
```
loess.model.1=loess(Mortality~Education,span=.25,degree=1)
loess.model.2=loess(Mortality~Education,span=.5,degree=1)
loess.model.3=loess(Mortality~Education,span=.7,degree=1)
loess.model.4=loess(Mortality~Education,span=.9,degree=1)
summary(loess.model.1)
## Call:
## loess(formula = Mortality ~ Education, span = 0.25, degree = 1)
## Number of Observations: 58
## Equivalent Number of Parameters: 7.85
## Residual Standard Error: 49.26
## Trace of smoother matrix: 9.33 (exact)
##
## Control settings:
##
     span
              : 0.25
##
     degree
                 1
##
     family
                 gaussian
##
     surface
                 interpolate
                                  cell = 0.2
##
     normalize:
                 TRUE
##
   parametric:
                 FALSE
## drop.square:
                 FALSE
summary(loess.model.2)
## Call:
## loess(formula = Mortality ~ Education, span = 0.5, degree = 1)
## Number of Observations: 58
## Equivalent Number of Parameters: 3.85
## Residual Standard Error: 49.02
## Trace of smoother matrix: 4.51
                                   (exact)
##
## Control settings:
##
     span
              :
                 0.5
##
     degree
                 1
##
     family
                 gaussian
                 interpolate
##
                                  cell = 0.2
     surface
##
     normalize:
                 TRUE
```

```
## parametric: FALSE
## drop.square: FALSE
summary(loess.model.3)
## Call:
## loess(formula = Mortality ~ Education, span = 0.7, degree = 1)
## Number of Observations: 58
## Equivalent Number of Parameters: 3.12
## Residual Standard Error: 48.58
## Trace of smoother matrix: 3.61 (exact)
##
## Control settings:
##
    span
            : 0.7
##
    degree : 1
##
    family : gaussian
##
    surface : interpolate
                              cell = 0.2
    normalize: TRUE
##
## parametric: FALSE
## drop.square: FALSE
summary(loess.model.4)
## Call:
## loess(formula = Mortality ~ Education, span = 0.9, degree = 1)
## Number of Observations: 58
## Equivalent Number of Parameters: 2.49
## Residual Standard Error: 48.21
## Trace of smoother matrix: 2.8 (exact)
##
## Control settings:
            : 0.9
##
    span
##
    degree
            : 1
##
    family
             : gaussian
##
    surface : interpolate
                                 cell = 0.2
    normalize: TRUE
##
## parametric: FALSE
## drop.square: FALSE
We will now plot the data points from our our mortality data,
plot(Mortality~Education)
```



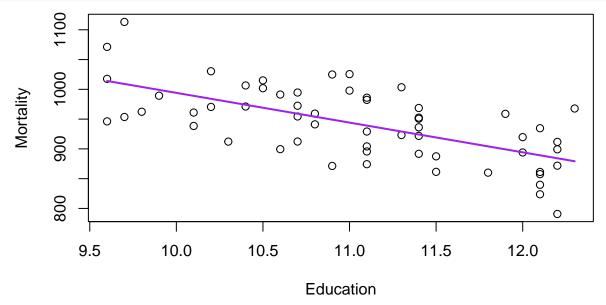
#The loess.smooth() function allows us to make fitted lines for the smoothed lines with varying
#We will plot various functions to be able to see the effect of span on the smoothing line
loessfit1=loess.smooth(x=Education,y=Mortality,span=.25,degree=1)
loessfit2=loess.smooth(x=Education,y=Mortality,span=.4,degree=1)
loessfit3=loess.smooth(x=Education,y=Mortality,span=.6,degree=1)
loessfit4=loess.smooth(x=Education,y=Mortality,span=.9,degree=1)

#Recall our plot with the mortality and education data. ****Needs legend*****
#We will now display the loess fits of varying span onto the plot to see the possible smoothing
plot(Mortality~Education)
lines(loessfit1\$x,loessfit1\$y,col="blue", lwd=2)
lines(loessfit2\$x,loessfit2\$y,col="green", lwd=2)
lines(loessfit3\$x,loessfit3\$y,col="yellow", lwd=2)
lines(loessfit4\$x,loessfit4\$y,col="red", lwd=2)



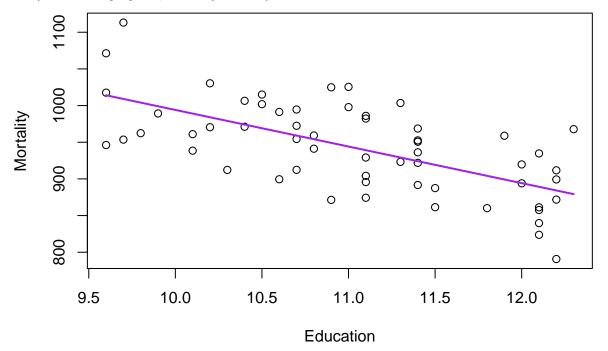
If we use 0.25 span for the case that it is the least jagged curve fit, while still holding some obvious grouping of values visually. One thing to keep note of is that the loess fit will be useful in visually displaying the relationship between the two variables mortality and education, but since our sample size is not particularly large, as loess fitting requires quite a large sample size to utilize effectively.

```
#Smoothing Spline Plot
plot(Mortality~Education)
spline.mortality=smooth.spline(Education, Mortality)
lines(spline.mortality, col="purple", lwd=2)
```



We can see that using a smoothing spline gives us a relatively linear line with small bumps along it.

4) Smoothing Spline, to the y-x data-fit.



We

can see that using a smoothing spline gives us a relatively linear line with small bumps along it. One thing to notice with the usage of the spline function in R is the ease with which one can apply the method through programs (e.g. R). With the spline function, we can see a fairly clear decreasing linear relationship between the two variables. This makes sense considering the spread of the original data on a scatterplot, but this also falls in line with the loess smoothing used prior. They both show a generally decreasing relationship between the response and predictor variables, but the varying spans in the loess function allow one to control the minute details within the data's distribution one might want to account for. Also, the smooth spline() function in 'R' is, similarly to usage in interpolating splines, defined through the use of a cubic spline in representing the fit of the model on the data.

Comparison for above Kernel Estimators: 1) the Nadaraya-Watson kernel estimator suffers from bias, both at the boundaries due to the one-sided neighborhoods and in the interior when the xi's are not uniformly distributed. The reason is that in local constant modeling more or less the same points are used to estimate the curve near the boundary. 2) Local polynomial regression overcomes the above problem by fitting a higher degree polynomial here. What's more, Local polynomial regression also has other advantage such as,independence of the regression design (fixed or random, highly clustered or nearly uniform), and efficiency in an asymptotic minimax sense.

Comparison for Kernel Estimators and Nearest neighbor methods: 1) In general, nearest neighbor and kernel estimators produce similar results. For example: The loess approach is similar to the Nadaraya-Watson approach in that both are taking linear combinations of the responses y_i

2) In terms of bias and variance, the nearest neighbor estimator performs well if the variance decreases more than the squared bias increases. For example: Suppose that f is continuously differentiable up to second order and that $K(x, x_0) = 0$ if $|x - x_0| > h$ Then Loess: $Biasf(x_0) = O(h^2)$

```
Nadaraya-Watson: Biasf(x_0) = f_0(x_0) \sum_i wi(x_i - x_0) + O(h^2), where w_i = K_h(x_i, x_0) / \sum_i K_h(x_i, x_0)
```

The leading term for the bias of the Nadaraya-Watson estimator is referred to as design bias which is not present for loess estimators. In other words, loess performs naturally eliminates design bias, and the resulting estimator is free of bias up to second order.

3) Nearest neighbor methods is better if we have spaces with clustered design points followed by intervals with sparse design points.

Comparison for Kernel Estimators, Nearest neighbor methods and spline regressions:

- 1) In general, for one input variable and one output variable, smoothing splines can basically do everything which kernel regression can do.
- 2) While a higher order polynomial will provide a closer fit at any particular point, the loss of parsimony is not the only potential problem of over fitting, unwanted oscillations can appear between data points. Spline functions avoid this pitfall.
 - 3) Kernels however are easier to program, analyze mathematically, extend more straightforwardly to multiple variables, and to combinations of discrete and continuous variables. Loess smoothing curves do not provide a particular mathematical formula to be applied for prediction, but rather are used for visual analysis of the data and its relationships.
- 4)Splines has faster computational speed and simplicity, as well as the clarity of controlling curvature directly.

3. Cross-Validation With the "Leave-One-Out" Procedure (10%):

Compare the above four methods with a leave-one-out cross-validation procedure.

4. Resampling Procedures: Bootstrap and Jackknife (25%):

- 1) Select an input x_0 in the [min(x-data), max(x-data)].
- 2) Use all four regression models built in Task #2 to make point-predictions of Y at x_0 .
- 3) Use both bootstrap (B = 1000) and jackknife resampling procedures to find a 90% pointwise confidence interval (CI) for the point-prediction. If the resampled distribution of the point-prediction is symmetric, use 5% in each tail to find the CI-bounds. If the distribution is not symmetric, use the HPD-interval idea to find the CI-bound. Compare the results from four regression methods.

Code Appendix

Problem 1

Exemplary code to produce pointwise confidence intervals, and confidence bands, based on the 'Hall-Wellner' methodology and implemented in the km.ci package in R: