Nonparametric Estimation

Statistics for Data Science CSE357 - Fall 2021

Nonparametric Estimation

Uses

- Data visualization and exploration
- Estimating a function without knowing function structure

How? examples...

- Kernel Density Estimation,
- Histograms
- Local regression (lowess, loess)
- Smoothing

Nonparametric Estimation

Why?

Besides tools for exploring data, can yield a deeper understand of the trade-offs at play with fitting a model to data.

Why?

Besides tooks for exploring data, can yield a deeper understand of the <u>trade-offs</u> at play with fitting a model to data.

Conceptually: As a model produces less <u>variance</u> (i.e. by penalizing the beta coefficients), it increases <u>bias</u>.

Conceptually: As a model produces less <u>variance</u> (i.e. by penalizing the beta coefficients), it increases <u>bias.</u>



too much bias: underfit

too much variance: overfit

Formally,

 \hat{g}_n -- estimator of true function, g (regression or density)

bias:
$$b(x)=\mathbb{E}({\hat g}_n(x))-g(x)$$
variance: $v(x)=\mathbb{V}({\hat g}_n(x))=\mathbb{E}(({\hat g}_n(x))-\mathbb{E}({\hat g}_n(x))^2)$

Formally,

 \hat{g}_n -- estimator of true function, g (regression or density)

Risk:
$$R(g, \hat{g}_n) = \int b^2(x) dx + \int v(x) dx$$
bias: $b(x) = \mathbb{E}(\hat{g}_n(x)) - g(x)$ variance: $v(x) = \mathbb{V}(\hat{g}_n(x)) = \mathbb{E}((\hat{g}_n(x)) - \mathbb{E}(\hat{g}_n(x))^2)$

$$egin{aligned} R(g,\hat{g}_n) &= \int b^2(x) dx + \int v(x) dx \ b(x) &= \mathbb{E}(\hat{g}_n(x)) - g(x) \ v(x) &= \mathbb{V}(\hat{g}_n(x)) = \mathbb{E}((\hat{g}_n(x)) - \mathbb{E}(\hat{g}_n(x))^2) \end{aligned}$$



FIGURE 20.2. The Bias-Variance trade-off. The bias increases and the variance decreases with the amount of smoothing. The optimal amount of smoothing, indicated by the vertical line, minimizes the risk = $bias^2 + variance$.

(Wasserman, 2005, AoS)

$$egin{aligned} R(g, \hat{g}_n) &= \int b^2(x) dx + \int v(x) dx \ b(x) &= \mathbb{E}(\hat{g}_n(x)) - g(x) \ v(x) &= \mathbb{V}(\hat{g}_n(x)) = \mathbb{E}((\hat{g}_n(x)) - \mathbb{E}(\hat{g}_n(x))^2 \end{aligned}$$



FIGURE 20.2. The Bias-Variance trade-off. The bias increases and the variance decreases with the amount of smoothing. The optimal amount of smoothing, indicated by the vertical line, minimizes the risk = $bias^2 + variance$.

(Wasserman, 2005, AoS)



Conceptually:

As a model produces less <u>variance</u> (i.e. by penalizing the beta coefficients), it increases <u>bias.</u>

Regression:
$$Y_i = r(x_i) + \epsilon_i$$

Nadaraya-Watson kernel estimator:

$$\hat{r} = \sum_{i=1}^n w_i(x) Y_i$$

where weights are given by (K is a kernel):

$$w_i(x) = rac{K(rac{x-x_i}{h})}{\sum_{j=1}^n K(rac{x-x_i}{h})}$$

(Wasserman)

Regression:
$$Y_i = r(x_i) + \epsilon_i$$

Nadaraya-Watson kernel estimator:

$$\hat{r} = \sum_{i=1}^n w_i(x) Y_i$$

where weights are given by (K is a kernel):





FIGURE 20.8. Regression analysis of the CMB data. The first fit is undersmoothed, the second is oversmoothed, and the third is based on cross-validation. The last panel shows the estimated risk versus the bandwidth of the smoother. The data are from BOOMERaNG, Maxima, and DASI. (Wasserman)

Regression:
$$Y_i = r(x_i) + \epsilon_i$$

Nadaraya-Watson kernel estimator:

$$\hat{r} = \sum_{i=1}^n w_i(x) Y_i$$

where weights are given by (K is a kernel):







Regression:
$$Y_i = r(x_i) + \epsilon_i$$

Local Linear Regression:

$$\hat{r}(x_0) = \hat{eta}_0(x_0) + \hat{eta}_1(x_0)x_0$$

Local Linear Regression at Boundary



Regression:
$$Y_i = r(x_i) + \epsilon_i$$

Local Linear Regression:



Local Linear Regression at Boundary



Regression:
$$Y_i = r(x_i) + \epsilon_i$$

Local Linear Regression:

$$\hat{r}(x_0) = {\hat{eta}}_0(x_0) + {\hat{eta}}_1(x_0)x_0$$

Objective: Minimize weighted least squares:

$$\sum_{i=1}^n K_\lambda(x_0,x_i) [y_i - eta_0(x_0) - eta_1(x_0)x_i]^2 \, .$$

Local Linear Regression at Boundary



Regression:
$$Y_i = r(x_i) + \epsilon_i$$

Local Linear Regression:

$$\hat{r}(x_0) = {\hat{eta}}_0(x_0) + {\hat{eta}}_1(x_0)x_0$$

Objective: Minimize weighted least squares:

$$\sum_{i=1}^n K_\lambda(x_0,x_i) [y_i - eta_0(x_0) - eta_1(x_0)x_i]^2 \, .$$

Full solution for local linear regression with normal equations for weighted least squares:

$$\hat{r}(x_0)=b(x_0)^T(eta^TW(x_0)eta)^{-1}eta^TW(x_0)y$$

Local Linear Regression at Boundary



Regression:
$$Y_i = r(x_i) + \epsilon_i$$

Local Linear Regression:

$$\hat{r}(x_0) = {\hat{eta}}_0(x_0) + {\hat{eta}}_1(x_0)x_0$$

Local Linear Regression at Boundary

00



1.5

Other Nonparametric Methods



Frequency

Kernel Density Estimation

#compute the bootstrap:

iters = 5000 #number of iterations
all_means = [] #will store the sample mean per iteration
#run the simulation loops:
for i in range(iters):
 resample = np.random.choice(sample, size=n, replace=True)
 resample_mean = resample.mean()
 all_means.append(resample_mean)

#sort the resampled means from least to greatest: sorted_means = sorted(all_means) #pick the upper and lower values for 95% CI: lower = sorted_means[int(0.025*iters)] upper = sorted_means[-int(0.025*iters)] print("95 CI based on the bootstrap: [%.3f, %.3f]" % (lower, upper))

95 CI based on the bootstrap: [19.239, 19.626]

The Bootstrap