STAT 824 hw 04

Orthogonal series estimator, backfitting, sparse backfitting, bootstrap

1. Suppose $\{\varphi_j\}_{j=1}^{\infty}$ is a basis for all functions $f : [0,1] \to \mathbb{R}$ such that $\int_0^1 |f(x)|^2 dx < \infty$ which satisfies

$$\int_0^1 \varphi_j(x)\varphi_{j'}(x)dx = \begin{cases} 1, & j = j' \\ 0, & j \neq j'. \end{cases} \tag{1}$$

A basis with the above property is called an *orthonormal basis.* Assume we can represent f as

$$f(x) = \sum_{i=1}^{\infty} \theta_j \varphi_j(x), \quad \text{where} \quad \theta_j = \int_0^1 f(x)\varphi_j(x)dx, \quad j = 1, 2, \dots$$

We will consider estimating the approximation $f_n^N(x) = \sum_{i=1}^N \theta_j \varphi_j(x)$ for some finite N in the context of nonparametric regression.

(a) Consider the *trigonometric basis*, which is given by $\varphi_1(x) = 1$, $\varphi_{2k}(x) = \sqrt{2}\cos(2\pi kx)$, and $\varphi_{2k+1}(x) = \sqrt{2}\sin(2\pi kx)$ for $k = 1, 2, \dots$ for $x \in [0,1]$. Show that this basis is orthonormal, i.e. that it satisfies 1.

(b) Let $(X_1, Y_1), \dots, (X_n, Y_n)$ be data pairs such that $Y_i = f(X_i) + \varepsilon_i$, where $X_i = i/n$, $i = 1, \dots, n$ and $\varepsilon_1, \dots, \varepsilon_n$ are independent with mean zero and variance $\sigma^2 < \infty$. Consider the estimator $\hat{f}_n^N$ of f given by

$$\hat{f}_n^N(x) = \sum_{j=1}^{N} \hat{\theta}_j \varphi_j(x), \quad \text{where} \quad \hat{\theta}_j = n^{-1} \sum_{i=1}^{n} Y_i \varphi_j(X_i), \quad j = 1, \dots, N. \tag{2}$$

This type of estimator is called an *orthogonal series estimator*. See [2] for more details.

i. For $x \in [0,1]$, find weights $W_{n1}(x), \dots, W_{nn}(x)$ such that $\hat{f}_n^N(x) = \sum_{i=1}^n W_{ni}(x) Y_i$.

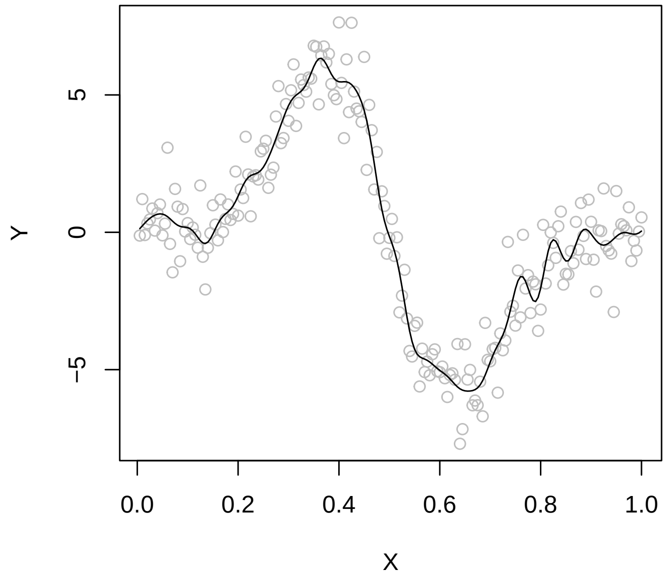
ii. Give the entries of the matrix $\mathbf{S}$ such that $\hat{\mathbf{f}}_n^N = \mathbf{S}\mathbf{Y}$, where $\hat{\mathbf{f}}_n^N = (\hat{f}_n^N(X_1), \dots, \hat{f}_n^N(X_n))^T$ and $\mathbf{Y} = (Y_1, \dots, Y_n)^T$.

iii. Give the matrix $\mathbf{B}$ such that $\mathbf{S} = (1/n)\mathbf{B}\mathbf{B}^T$.

iv. Generate data with the R code

```
m <- function(x){ - 25 * 4 * (2*x - 1) * dnorm(4*(2*x - 1))}
n <- 200
X <- c(1:n)/n
Y <- m(X) + rnorm(n,0,1)
```

Then make a scatterplot of the data with a curve overlaid which traces the fitted values $\hat{f}_n^N(X_1), \dots, \hat{f}_n^N(X_n)$ of the estimator in (2) based on the trigonometric basis with functions for $k = 1, \dots, 20$, such that $N = 41$. My plot looks like this:



v. What do you notice about the quantities $n^{-1}\sum_{i=1}^{n}\varphi_j(i/n)\varphi_{j'}(i/n)$, $1 \le j, j' \le N$, in relation to the property in (1)? *Hint: These are the entries of the matrix* $(1/n)\mathbf{B}^T\mathbf{B}$*, which you can compute in R.*

vi. Now consider using the trigonometric basis with functions for $k = 1, \ldots, K$, giving $N = 2K+1$ total basis functions: Choose K via leave-one-out crossvalidation (note that you can use the special trick for linear estimators to save computation time). Report the chosen value of K and the corresponding number of basis functions N. Also make a scatterplot of the data with the curve tracing the fitted values overlaid.

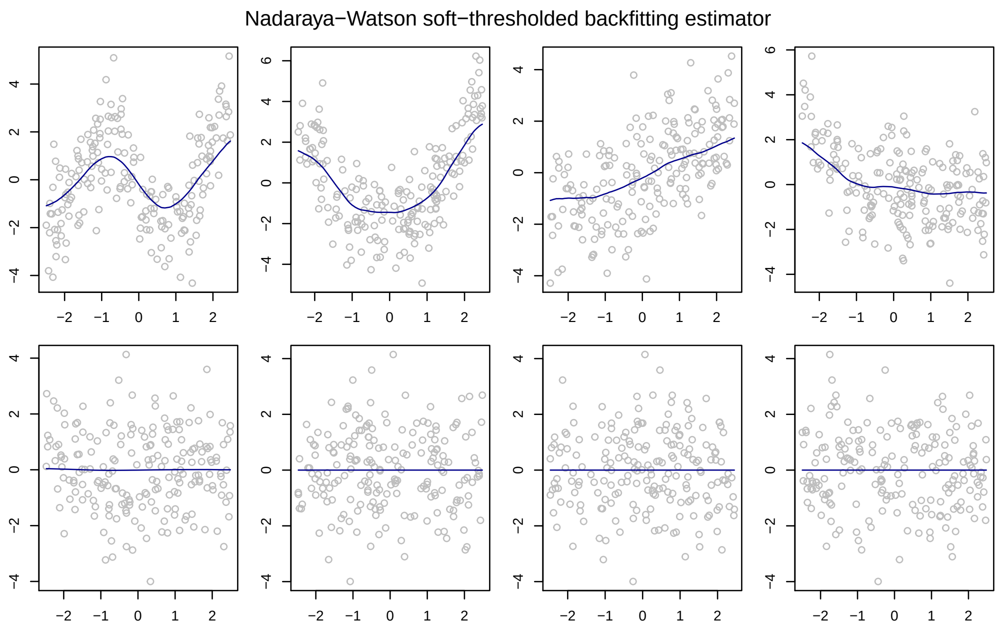
2. Import into R the data in [this `.Rdata` file] and fit the additive model

$$Y = \mu + m_1(X_1) + \cdots + m_8(X_8) + \varepsilon$$

with a soft-thresholded (sparse) Nadaraya-Watson backfitting estimator, enforcing the usual identifiability condition on the additive components.

(a) Give $\hat{\mu}$.

(b) Make a plot like the one pictured below (choose a bandwidth h and a soft-thresholding parameter just by eyeballing the plot), where in panel j, the points $(Y_i - \sum_{k\neq j}\hat{m}_k(X_{ik}), X_{kj})$, $i = 1, \ldots, n$, are plotted along with a line tracing the fitted values $\hat{m}_j(X_{ij})$, $i = 1, \ldots, n$.



(c) Now fit Nadaraya-Watson backfitting estimator *without* soft-thresholding; make a similar plot.

3. Let $(X_1, Y_1), \dots, (X_n, Y_n)$ be iid realizations of (X, Y). Let $\rho = \text{corr}(X, Y)$ and $\hat{\rho}$ be the sample correlation. If (X, Y) are bivariate Normal then $\sqrt{n}(\zeta(\hat{\rho}) - \zeta(\rho)) \xrightarrow{\text{D}} \text{Normal}(0, 1)$ as $n \to \infty$ where

$$\zeta(\rho) = \frac{1}{2} \log\left(\frac{1+\rho}{1-\rho}\right).$$

(a) Let $Y|X \sim \text{Normal}(\rho X, 1-\rho^2)$, $X \sim \text{Normal}(0,1)$ so that (X, Y) are bivariate standard Normal with correlation ρ. For $\alpha = 0.05$, $n = 50$, $\rho = 1/2$, and $B = 500$, run a simulation with 500 simulated data sets to compare the coverage of ρ and the average width of the three intervals

$$\begin{aligned}
\mathcal{A}_n &= [\zeta^{-1}(\zeta(\hat{\rho}) - n^{-1/2} z_{\alpha/2}), \zeta^{-1}(\zeta(\hat{\rho}) + n^{-1/2} z_{\alpha/2})] \\
\mathcal{B}_n^{\text{pctl}} &= [\hat{\rho}_n^{*((\alpha/2)B)}, \hat{\rho}_n^{*((1-\alpha/2)B)}] \\
\mathcal{B}_n^{\text{piv}} &= [\zeta^{-1}(2\hat{\zeta}_n - \hat{\zeta}_n^{*((1-\alpha/2)B)}), \zeta^{-1}(2\hat{\zeta}_n - \hat{\zeta}_n^{*((\alpha/2)B)})],
\end{aligned}$$

where $\zeta^{-1}(z) = \frac{e^{2z}-1}{e^{2z}+1}$, $\hat{\rho}_n^{*(1)} \le \dots \le \hat{\rho}_n^{*(B)}$ are sorted bootstrap realizations of $\hat{\rho}$ from samples drawn with replacement from $(X_1, Y_1), \dots, (X_n, Y_n)$, and $\hat{\zeta}_n^{*(b)} = \zeta(\hat{\rho}_n^{*(b)})$ for $b = 1, \dots, B$ with $\hat{\zeta}_n = \zeta(\hat{\rho}_n)$.

(b) Now let $Y|X \sim \text{Normal}(X, \sigma^2)$, $X \sim \text{Exponential}(\lambda)$ with $\lambda = 1$ and $\sigma^2 = 3$. Find $\rho = \text{corr}(X, Y)$ and compare the coverage of ρ and the width of the intervals for $\alpha = 0.05$, $n = 50$, and $B = 500$ as before.

(c) Why does the asymptotic interval $\mathcal{A}_n$ perform poorly under the settings in part (b)?

(d) Which interval performed best in parts (a) and (b)?

4. (Optional) Let $\mathbf{X} \in \mathbb{R}^{n \times p}$, $p < n$, be a full-rank matrix and let $\mathbf{Y} \in \mathbb{R}^n$ and partition the columns of $\mathbf{X}$ such that $\mathbf{X} = [\mathbf{X}_1, \mathbf{X}_{-1}]$. Let $\hat{\boldsymbol{\beta}} \in \mathbb{R}^p$ be the vector such that $(\mathbf{X}^T\mathbf{X})\hat{\boldsymbol{\beta}} = \mathbf{X}^T\mathbf{Y}$ and let $\hat{\boldsymbol{\beta}}$ be partitioned in the same way as $\mathbf{X}$ into

$$\hat{\boldsymbol{\beta}} = \begin{bmatrix} \hat{\boldsymbol{\beta}}_1 \\ \hat{\boldsymbol{\beta}}_{-1} \end{bmatrix}.$$

Define $\mathbf{P}_1 = \mathbf{X}_1(\mathbf{X}_1^T\mathbf{X}_1)^{-1}\mathbf{X}_1^T$ and $\mathbf{P}_{-1} = \mathbf{X}_{-1}(\mathbf{X}_{-1}^T\mathbf{X}_{-1})^{-1}\mathbf{X}_{-1}^T$, and let $\mathbf{X}_{1\backslash -1} = (\mathbf{I} - \mathbf{P}_{-1})\mathbf{X}_1$ be the residuals from regressions of the columns of $\mathbf{X}_1$ onto the columns of $\mathbf{X}_{-1}$.

(a) Let $\hat{\mathbf{Y}}_1 = \mathbf{X}_1\hat{\boldsymbol{\beta}}_1$ and let $\hat{\mathbf{Y}}_{-1} = \mathbf{X}_{-1}\hat{\boldsymbol{\beta}}_{-1}$.

i. Show that the normal equations $(\mathbf{X}^T\mathbf{X})\hat{\boldsymbol{\beta}} = \mathbf{X}^T\mathbf{Y}$ are equivalent to

$$\hat{\mathbf{Y}}_1 = \mathbf{P}_1(\mathbf{Y} - \hat{\mathbf{Y}}_{-1})$$
$$\hat{\mathbf{Y}}_{-1} = \mathbf{P}_{-1}(\mathbf{Y} - \hat{\mathbf{Y}}_1).$$

ii. Show that

$$\begin{pmatrix} \mathbf{I} & \mathbf{P}_1 \\ \mathbf{P}_{-1} & \mathbf{I} \end{pmatrix} \begin{pmatrix} \hat{\mathbf{Y}}_1 \\ \hat{\mathbf{Y}}_{-1} \end{pmatrix} = \begin{pmatrix} \mathbf{P}_1\mathbf{Y} \\ \mathbf{P}_{-1}\mathbf{Y} \end{pmatrix}.$$

(b) Show that $\hat{\mathbf{Y}}_1 = (\mathbf{I} - \mathbf{P}_1\mathbf{P}_{-1})^{-1}\mathbf{P}_1(\mathbf{I} - \mathbf{P}_{-1})\mathbf{Y}$.

(c) The Gauss–Seidel or backfitting algorithm for finding $\hat{\mathbf{Y}}_1$ and $\hat{\mathbf{Y}}_{-1}$ is the following:

Initialize $\hat{\mathbf{Y}}_1 \leftarrow \mathbf{0}$ and $\hat{\mathbf{Y}}_{-1} \leftarrow \mathbf{0}$. Then repeat the steps

i. $\hat{\mathbf{Y}}_1 \leftarrow \mathbf{P}_1(\mathbf{Y} - \hat{\mathbf{Y}}_{-1})$
ii. $\hat{\mathbf{Y}}_{-1} \leftarrow \mathbf{P}_{-1}(\mathbf{Y} - \hat{\mathbf{Y}}_1)$

until $\hat{\mathbf{Y}}_1$ and $\hat{\mathbf{Y}}_{-1}$ do not change.

Show that in the kth iteration of the backfitting algorithm, we have

$$\hat{\mathbf{Y}}_1^{(k)} \leftarrow \left[\mathbf{I} - \textstyle\sum_{l=0}^{k-1}(\mathbf{P}_1\mathbf{P}_{-1})^l(\mathbf{I} - \mathbf{P}_1)\right]\mathbf{Y}.$$

(d) Show that

$$\mathbf{I} - \sum_{l=0}^{\infty}(\mathbf{P}_1\mathbf{P}_{-1})^l(\mathbf{I} - \mathbf{P}_1) = (\mathbf{I} - \mathbf{P}_1\mathbf{P}_{-1})^{-1}\mathbf{P}_1(\mathbf{I} - \mathbf{P}_{-1}),$$

in consequence of which $\hat{\mathbf{Y}}_1^{(k)} \to \hat{\mathbf{Y}}_1$ as $k \to \infty$. You will make use of the fact that for any real-valued square matrix $\mathbf{A}$, $\mathbf{I} + \mathbf{A} + \mathbf{A}^2 + \cdots = (\mathbf{I} - \mathbf{A})^{-1}$, provided $\lambda_{\max}(\mathbf{A}^T\mathbf{A}) < 1$, and you may assume $\lambda_{\max}(\mathbf{P}_1\mathbf{P}_{-1}\mathbf{P}_1) < 1$.

References

[1] John F Monahan. *A primer on linear models*. CRC Press, 2008.

[2] Alexandre B Tsybakov. *Introduction to nonparametric estimation*. Springer Science & Business Media, 2008.