## STAT 824 sp 2023 Lec 05 slides

# Nonparametric regression: Least-squares splines 

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These slides are an instructional aid; their sole purpose is to display, during the lecture, definitions, plots, results, etc. which take too much time to write by hand on the blackboard.

They are not intended to explain or expound on any material.

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(1) Least-squares nonparametric regression estimators
(2) Splines and rates of convergence for least squares splines
(3) B-splines as basis functions
(4) Sketch of proof of mean squared error bound

Let $\left(X_{1}, Y_{1}\right), \ldots,\left(X_{n}, Y_{n}\right)$ be indep. realizations of $(X, Y) \in[0,1] \times \mathbb{R}$, where

$$
Y=m(X)+\varepsilon, \quad \text { for some } m:[0,1] \rightarrow \mathbb{R},
$$

where $\varepsilon$ is independent of $X$ with $\mathbb{E} \varepsilon=0$ and $\mathbb{E} \varepsilon^{2}=\sigma^{2}$.

Idea: Given a set of basis functions $b_{1}, \ldots, b_{d_{n}}:[0,1] \rightarrow \mathbb{R}$, suppose

$$
m(x) \approx \sum_{k=1}^{d_{n}} \alpha_{k} b_{k}(x) \quad \text { for some } \quad \alpha_{1}, \ldots, \alpha_{d_{n}}
$$

Then estimate $\alpha_{1}, \ldots, \alpha_{d_{n}}$ with least squares to get $\hat{m}_{n}(x)=\sum_{k=1}^{d_{n}} \hat{\alpha}_{k} b_{k}(x)$.

- As $n \rightarrow \infty$, let $d_{n} \rightarrow \infty$ so that the approximation improves.
- Quality of approximation depends on
(1) the type and number of basis functions.
(2) the smoothness of the true function $m$.
- There will always be some approximation bias.


## A non-parametric least squares estimator

For a set of basis functions $b_{1}, \ldots, b_{d_{n}}:[0,1] \rightarrow \mathbb{R}$, let

$$
\mathcal{B}_{n}=\left\{m: m(x)=\sum_{k=1}^{d_{n}} \alpha_{k} b_{k}(x), \alpha_{1}, \ldots, \alpha_{d_{n}} \in \mathbb{R}\right\} .
$$

Given $\left(X_{1}, Y_{1}\right), \ldots,\left(X_{n}, Y_{n}\right)$, the least squares estimator of $m$ in $\mathcal{B}_{n}$ is given by

$$
\hat{m}_{n}=\underset{g \in \mathcal{B}_{n}}{\operatorname{argmin}} \sum_{i=1}^{n}\left[Y_{i}-g\left(X_{i}\right)\right]^{2} .
$$

Exercise: Let $\mathbf{Y}=\left(Y_{1}, \ldots, Y_{n}\right)^{T}$ and define the matrix

$$
\mathbf{B}=\left(b_{k}\left(X_{i}\right)\right)_{1 \leq i \leq n, 1 \leq k \leq d_{n}} .
$$

Show that $\hat{m}_{n}(x)=\mathbf{b}_{x}^{T} \hat{\boldsymbol{\alpha}}$, where

$$
\hat{\boldsymbol{\alpha}}=\left(\mathbf{B}^{T} \mathbf{B}\right)^{-1} \mathbf{B}^{T} \mathbf{Y} \quad \text { and } \quad \mathbf{b}_{x}=\left(b_{1}(x), \ldots, b_{d_{n}}(x)\right)^{T} .
$$

$$
\begin{aligned}
& \left(x_{1}, y_{1}\right) \ldots\left(x_{n}, y_{n}\right) . \\
& \sum_{i=1}^{n}\left(y_{i}-\gamma_{T_{d n}}\left(x_{i}\right)\right)^{2}=\sum_{i=1}^{n}\left(Y_{i}-\sum_{j=1}^{d_{n}} \alpha_{j} b_{j}\left(x_{i}\right)\right)^{2}=(\underset{\sim}{y}-\mathbb{B} \underset{\sim}{\alpha})^{\top}\left(\underset{\sim}{y}-\mathbb{B}_{\underline{\alpha}}\right) \\
& \sum_{i=1}^{d_{n}} \alpha_{j} b_{j}\left(X_{i}\right)=\|\underbrace{\|}_{n \times 1}-B_{\alpha}\|_{2}^{2} \\
& \underset{n \times d_{n}}{\mathbb{B}}=\left[\begin{array}{cccc}
b_{1}\left(x_{1}\right) & b_{2}\left(x_{1}\right) & \cdots & b_{d_{n}}\left(x_{1}\right) \\
\vdots & \vdots & & \vdots \\
b_{1}\left(x_{n}\right) & b_{2}\left(x_{n}\right) & & b_{d}\left(x_{n}\right)
\end{array}\right] \quad d=\left(\begin{array}{c}
d_{1} \\
\vdots \\
d_{d_{n}}
\end{array}\right) \\
& \underset{n r 1}{\underset{y}{y}}=\left(\begin{array}{c}
y_{1} \\
\vdots \\
y_{n}
\end{array}\right)
\end{aligned}
$$

$$
\begin{aligned}
& \hat{m}_{n}\left(x_{0}\right)=\sum_{j=1}^{d} \hat{d}_{j} b_{i}\left(x_{0}\right)=\underset{\sim x_{0}}{b_{j}^{\top}} \hat{\underset{d}{e}} \\
& \underset{\sim}{b_{0}}=\left[\begin{array}{c}
b_{1}\left(x_{0}\right. \\
\vdots \\
b_{d}\left(x_{0}\right)
\end{array}\right]
\end{aligned}
$$

## Splines: see Stone (1985) [2]

For a positive integer $K_{n}$ let


$$
I_{n k}=\left[\frac{k-1}{K_{n}}, \frac{k}{K_{n}}\right), \quad k=1, \ldots, K_{n}-1, \quad \text { and } \quad I_{n K_{n}}=\left[\frac{K_{n}-1}{K_{n}}, 1\right] .
$$

For $r \geq 1$, define the set of functions

$$
\mathcal{M}_{n, r}=\left\{\begin{array}{ll}
m:[0,1] \rightarrow \mathbb{R}: \begin{array}{l}
m \text { is a polynomial of degree } r \text { or less on } \\
\text { each interval } I_{1}, \ldots, I_{n K_{n}}, \\
\text { and } m \text { is } r-1 \text { times } \\
\text { continuously differentiable on }[0,1]
\end{array}
\end{array}\right\} .
$$

Moreover, let

$$
\mathcal{M}_{n, 0}=\left\{m:[0,1] \rightarrow \mathbb{R}: m \text { is piecewise constant on } I_{1}, \ldots, I_{n K_{n}}\right\}
$$

- Fns in $\mathcal{M}_{n, 1}, \mathcal{M}_{n, 2}$, and $\mathcal{M}_{n, 3}$ are called linear, quadratic, and cubic splines.
- Values $j / K_{n}, j=0, \ldots, K_{n}$ are called knots. Can choose knots differently.
- Functions in these spaces can nicely approximate functions in Hölder classes.

For a function $g: \mathcal{T} \rightarrow \mathbb{R}$, we write $\|g\|_{\infty}=\sup _{x \in \mathcal{T}}|g(x)|$.

## Key result from deBoor (1968) [1]

For each $m \in \mathcal{H}(\beta, L)$
$r \geq \beta-1$ such that on $[0,1]$, there exists a functior $m_{n, r}^{\text {spl } \in \mathcal{M}_{n, r},}$ where

$$
\left\|m-m_{n, r}^{\mathrm{spl}}\right\|_{\infty} \leq C \cdot K_{n}^{-\beta}
$$

for some constant $C>0$.

Idea is to let $K_{n} \rightarrow \infty$ as $n \rightarrow \infty$, so that this approximation error goes to zero.
Exercise: For $m \in \operatorname{Lipschitz}(L)$ on $[0,1]$, show that $\exists m_{n, 0}^{\text {spl }} \in \mathcal{M}_{n, 0}$ such that $\left|m(x)-m\left(x^{\prime}\right)\right| \leq L\left|x-x^{\prime}\right|$

$$
\sup _{x \in[0,1]}\left|m(x)-m_{n, 0}^{\mathrm{spl}}(x)\right| \leq \frac{L}{K_{n}}
$$

$$
\begin{aligned}
& m_{n=0}^{s-1}(x)=m\left(\frac{k-1}{k_{n}}\right) \quad \text { f.. } \quad x \in\left(\frac{k-1}{k_{n}}, \frac{k}{k_{n}}\right) \quad k=1, \ldots k .
\end{aligned}
$$

$$
\begin{aligned}
& \begin{array}{l}
=\max _{1 \leq k \leq k_{n}} \sin _{x \in\left[\frac{k-1}{k_{n}}, \frac{k}{k_{n}}\right]} \underbrace{\left.\ln (x)--\frac{k-1}{k_{n}}\right) \mid}_{\leq \frac{L}{k_{n}}} \\
\quad \leq L .
\end{array} \\
& \leq \frac{\llcorner }{k_{-}} \text {. } \\
& K_{n}= \pm \text { intan's }
\end{aligned}
$$

Reall: MSE $m_{n}^{N \omega}(x) \leq C\left(h^{2 \beta}+\frac{1}{n h}\right)$

We now define the order $r$ least-squares splines estimator of $m$ as

$$
\hat{m}_{n, r}^{\text {sp }}=\underset{g \in \mathcal{M}_{n, r}}{\operatorname{argmin}} \sum_{i=1}^{n}\left[Y_{i}-g\left(X_{i}\right)\right]^{2} .
$$

Bound on MSE $\hat{m}_{n, r}^{\mathrm{spl}}\left(x_{0}\right)$
$K_{n}$ is lite $\frac{1}{n}$
If $m \in \mathcal{H}(\beta, L)$ on $[0,1]$, then for $r \geq \beta-1$, we have

$$
\operatorname{MSE} \hat{m}_{n, r}^{\mathrm{spl}}\left(x_{0}\right) \leq C \cdot\left(K_{n}^{-2 \beta}+\frac{K_{n}}{n}\right)
$$

for all $x_{0} \in[0,1]$ for large enough $n$, provided (C1), (C2), and (C3) hold.

We will study the conditions (C1), (C2), and (C3) later on.

## Exercise:

(3) Find the value of $K_{n}$ which minimizes the MSE bound.
(2) Give the minimum bound over choices of $K_{n}$.
(3) Anything interesting about this?

For our spline spaces $\mathcal{M}_{n, r}$, we need sets of basis functions $b_{1}, \ldots, b_{d_{n}}$ such that

$$
\mathcal{M}_{n, r}=\left\{m:[0,1] \rightarrow \mathbb{R}: m=\sum_{k=1}^{d_{n}} \alpha_{k} b_{k}, \alpha_{1}, \ldots, \alpha_{d_{n}} \in \mathbb{R}\right\} .
$$

## B-splines: Cox-deBoor recursion formula

For a non-decreasing set of knots $0=u_{0} \leq u_{1} \leq \cdots \leq u_{K}=1$, let

$$
N_{k, 0}(u)=\left\{\begin{array}{ll}
\frac{1}{0}, & u_{k} \leq u<u_{k+1} \\
0, & \text { otherwise }
\end{array} \quad \text { for } k=0, \ldots, K-1,\right.
$$

and

$$
N_{k, r}(u)=\frac{u-u_{k}}{u_{k+r}-u_{k}} N_{k, r-1}(u)+\frac{u_{k+r+1}-u}{u_{k+r+1}-u_{k+1}} N_{k+1, r}(u)
$$

for $k=0, \ldots, K-r-1$. These functions are called $B$-splines.
Can compute row vector $\mathbf{N}_{r}(x)=\left(N_{0, r}(x), \ldots, N_{K-r-1, r}(x)\right), x \in[0,1]$, with

$$
\text { splineDesign(knots }=u, x=x \text {, ord }=r+1 \text { ) }
$$

Require splines package.

The Cox-deBoor recursion has a structure like this:


Exercise: Show construction of $N_{0,1}$ based on knots $\left(u_{0}, u_{1}, u_{2}\right)=(0,1 / 2,1)$.



To handle boundary issues, a convention is to include the end knots r+1

$$
0=u_{-r}=\cdots=u_{0}<u_{1}<\cdots<u_{K}=\cdots=u_{K+r}
$$

This results in $K+r$ basis functions when $[0,1]$ is subdivided into $K$ intervals.

Exercise: Make beautiful plots of B -spline functions of order $r=0,1,2,3$ in R
(1) with equally spaced knots.
(2) with unequally spaced knots.


B-splines of order $r=1$




Replicating boundary knots $r$ times results in $d_{n}=K_{n}+r$ basis functions.

For $X_{1}, \ldots, X_{n}$, we can obtain the $n \times d_{n}$ design matrix $\mathbf{B}$ with

$$
\text { splineDesign(knots }=u, x=X, \text { ord }=r+1),
$$

where X is a vector containing the values $X_{1}, \ldots, X_{n}$.

Note that (with the replicated boundary knots) the rows of $\mathbf{B}$ always sum to 1 .

## Exercise:

(1) For $n=200$, generate data $Y_{i}=m\left(X_{i}\right)+\varepsilon_{i}$ with

- $X_{1}, \ldots, X_{n} \stackrel{\text { ind }}{\sim} \operatorname{Uniform}(0,1)$, indep. of $\varepsilon_{1}, \ldots, \varepsilon_{n} \stackrel{\text { ind }}{\sim} \operatorname{Normal}(0,1)$
- $m(x)=5 x \cdot \sin \left(2 \pi(1+x)^{2}\right)$
(2) Plot $\hat{m}_{n, r}^{\text {spl }}$ under $K_{n}=10$ for $r=0,1,2,3$ with
- knots equally spaced in $[0,1]$
- knots at equally space quantiles of $X_{1}, \ldots, X_{n}$
(3) Try different values of $K_{n}$.

With B-splines of order $r=0$


With B-splines of order $\mathrm{r}=2$


With B-splines of order $r=1$



With B-splines of order $r=0$



With $B$-splines of order $r=1$



With B-splines of order $r=0$


With B-splines of order $r=2$


With B-splines of order $r=1$



With B-splines of order $r=0$



With $B$-splines of order $r=1$


## Conditions for bounding MSE $\hat{m}_{n, r}^{\text {spl }}\left(x_{0}\right)$; see Zhou (1998) [3]

Let $m \in \mathcal{H}(\beta, L)$ on $[0,1]$ and let $m_{n, r}^{\text {spl }} \in \mathcal{M}_{n, r}$ satisfy $\left\|m-m_{n, r}^{\text {spl }}\right\|_{\infty} \leq C \cdot K_{n}^{-\beta}$. Let $X_{1}, \ldots, X_{n} \in[0,1]$ be deterministic such that for large enough $n$,
(C1) $K_{n}^{-1} \cdot c_{1} \leq \lambda_{\text {min }}\left(n^{-1} \mathbf{B}^{T} \mathbf{B}\right) \leq \lambda_{\text {max }}\left(n^{-1} \mathbf{B}^{T} \mathbf{B}\right) \leq C_{1} \cdot K_{n}^{-1}$
(C2) $\left\|\left(n^{-1} \mathbf{B}^{\top} \mathbf{B}\right)^{-1}\right\|_{\infty} \leq C_{2} \cdot K_{n}$
(C3) $\left\|n^{-1} \mathbf{B}^{T}\left(\mathbf{m}-\mathbf{m}_{n, r}^{\text {spl }}\right)\right\|_{\infty} \leq C_{3} \cdot K_{n}^{-1-\beta}$,
where

$$
\mathbf{m}=\left(m\left(X_{1}\right), \ldots, m\left(X_{n}\right)\right)^{T} \quad \text { and } \quad \mathbf{m}_{n, r}^{\text {spl }}=\left(m_{n, r}^{\text {spl }}\left(X_{1}\right), \ldots, m_{n, r}^{\text {spl }}\left(X_{n}\right)\right)^{T} .
$$

## Exercise:

(1) Use above to get bounds on the bias and variance of $\hat{m}_{n, r}^{\text {spl }}\left(x_{0}\right)$.
(2) Consider (C1), (C2), and (C3) in the case of $\beta=1, r=0$.

Idee:

$$
\begin{array}{r}
Y_{i}=m\left(X_{i}\right)+\varepsilon_{i}, \quad i=1, \ldots, n, \quad \varepsilon_{1} \ldots \varepsilon_{1} i^{l} N(0 \\
m(x) \approx \sum_{j=1}^{d} \alpha_{j} b_{j}(x)
\end{array}
$$



$$
\begin{aligned}
& \left(\hat{\alpha}_{1, \ldots,}, \hat{\alpha}_{d}\right)=\operatorname{orgmin}_{\alpha_{1}, \ldots, \alpha_{d}} \\
& Y_{i}-\sum_{j=1}^{d} \alpha_{j} b_{j}\left(x_{i}\right) \\
& {\left[\begin{array}{cc}
Y_{1} & - \\
\sum_{i=1}^{d} d_{j} b_{j}\left(X_{1}\right) \\
\vdots & \\
Y_{n} & -\sum_{j=1}^{d} d_{j} b_{j}\left(X_{n}\right)
\end{array}\right]=\left[\begin{array}{l}
Y_{1} \\
Y_{n}
\end{array}\right]-\left[\begin{array}{l}
\sum_{j=1}^{d} d_{j} b_{j}\left(X_{1}\right) \\
\sum_{j=1}^{d} d_{j} b_{j}\left(X_{n}\right)
\end{array}\right]} \\
& =\left[\begin{array}{l}
y_{1} \\
y_{n}
\end{array}\right]-\left[\begin{array}{cc}
\alpha_{1} b_{1}\left(x_{1}\right)+ & +\alpha_{d} b_{d}\left(x_{1}\right) \\
\\
\alpha_{1} b_{1}\left(x_{n}\right)+ & \cdots
\end{array}\right] \\
& =\left[\begin{array}{l}
y_{1} \\
\\
y_{n}
\end{array}\right]-\left[\begin{array}{ccc}
b_{1}\left(x_{1}\right) & \cdots & b_{d}\left(x_{1}\right) \\
\vdots & \ddots & \vdots \\
b_{1}\left(x_{n}\right) & \cdots & b_{d}\left(x_{n}\right)
\end{array}\right]\left[\begin{array}{l}
\alpha_{1} \\
\\
\alpha_{d}
\end{array}\right] \\
& =\underset{\sim}{\sim}-\mathbb{B} \underset{\sim}{\alpha}
\end{aligned}
$$

The

$$
\begin{aligned}
& \underset{\text { der }}{\hat{\alpha}}=\underset{\alpha}{\operatorname{argume}}\|\underline{\sim}-\mathbb{B} \underline{\underline{Q}}\|_{2}^{2}=\left(B^{\top} B\right)^{-1} \mathbb{B}^{\top} \underline{\sim}
\end{aligned}
$$


wher

$$
\underset{\sim}{b_{x_{0}}}=\left(\begin{array}{c}
b_{1}\left(x_{0}\right) \\
\vdots \\
b_{d}\left(x_{0}\right)
\end{array}\right) .
$$

$r=o o d r$
An.lysis of Vrima al bies of $\hat{m}_{n, r}^{\text {spl }}\left(x_{0}\right)$.

$$
\begin{aligned}
& V_{C}\left[\hat{m}_{m, c}^{n_{r 1}\left(x_{0}\right)}\right]=V_{r}\left[\begin{array}{ll}
b_{x_{0}}{ }^{\top} & \hat{\alpha}
\end{array}\right] \\
& \operatorname{Var}\left(c^{\top} x\right) \quad=\operatorname{Vr}[\underbrace{b_{n}^{\top}\left(B^{\top} B\right)^{-1} B^{\top}}_{1 \times n} \underset{n \times 1}{Y}] \\
& =s^{\top} \cos (\underline{x}) \leq \quad=b_{x}^{\top}\left(\mathbb{B}^{\top} B\right)^{-1} \mathbb{B}^{\top} \underbrace{\operatorname{cov}(\underline{I})}_{\sigma^{2} I_{n}} \mathbb{B}\left(B^{\top} B\right)^{-1} h_{x_{0}}
\end{aligned}
$$

$$
\begin{aligned}
& \frac{1}{n} X_{n \times r}^{\top} X \rightarrow \Sigma \quad \leq \frac{\sigma^{2}}{n} S_{m \ldots}\left(\left(\frac{1}{n} \beta^{\top} B\right)^{-1}\right)\left\|h_{m_{0}}\right\|_{2}^{2} \\
& \leq \frac{\sigma^{2}}{n} \frac{1}{\operatorname{Sin}\left(\frac{1}{n} B^{\top} B\right)} \underbrace{\left\|b_{n}\right\|_{2}^{2}}_{\varepsilon_{1}}
\end{aligned}
$$

$$
\begin{aligned}
& \Lambda_{\text {max }}(A)=\frac{1}{\Lambda_{\text {min }}}\left(A^{-1}\right) \quad \leq \frac{\sigma^{2}}{n} \frac{K_{n}}{c_{1}} . \\
& A=Q \Delta Q^{\top}, \quad Q Q^{\top}=Q^{\top} Q=I \\
& A^{-1}=Q S^{-1} Q^{\top} \text {, bean } \\
& Q S^{-1} \underbrace{Q^{\top} Q}_{I} \Delta Q^{\top} \\
& \operatorname{Vr}\left[\hat{m}_{n, r}^{s s_{1}}\left(x_{0}\right)\right] \leq \frac{\sigma^{2}}{n} \frac{K_{n}}{c_{1}} \\
& =Q s^{-1} \Delta Q^{\top} \\
& =Q Q^{\top}=\Sigma \text {. } \\
& V_{C}\left[\hat{\omega}_{n}^{N \omega}\left(x_{0}\right)\right]=\frac{\sigma^{2}}{n h} C
\end{aligned}
$$

What don $\quad \Lambda_{\text {min }}\left(\frac{1}{n} B^{T} B\right) \geq \frac{c_{1}}{k}$ men ?
Constr $r=0$ case. The $b_{j}(x)=\mathbb{Z}\left(\frac{j-1}{k} \leq x<\frac{j-1}{k}\right) \quad j=1, \ldots k$,

$$
=\mathbb{Z}(x \in I ;) \quad k=d .
$$

The $\quad \frac{1}{n} B^{\top} B=$ ?

Wall

$$
\begin{aligned}
& B=\left[\begin{array}{ccc}
b_{1}\left(x_{1}\right) & \cdots & b_{d}\left(x_{1}\right) \\
\vdots & \ddots & \vdots \\
b_{1}\left(x_{n}\right) & \cdots & b_{n}\left(x_{n}\right)
\end{array}\right]=\left[\begin{array}{ccc}
\mathbb{Z}\left(x_{1} \in I_{2}\right) & \cdots & \mathbb{Z}\left(x_{1} \subset I_{d}\right) \\
\vdots & & \\
\mathbb{Z}\left(x_{n} \in I_{2}\right) & \cdots \mathbb{Z}\left(x_{n} \in I_{a}\right)
\end{array}\right]
\end{aligned}
$$

$$
\begin{aligned}
& =\left[\begin{array}{lll}
\frac{\#\left\{x_{i} \in I_{1}\right\}}{n} & & \\
& \ddots & \\
& & \frac{\#\left\{x_{i} \in I_{d}\right\}}{n}
\end{array}\right] \\
& \Delta_{m i n}\left(\frac{1}{n} \mathbb{B}^{\top} \mathbb{B}\right)=\min _{1 \leq k \leq d} \frac{\boldsymbol{y} \quad \frac{x_{i} \in I_{n} \xi}{n} \geqslant \frac{c_{1}}{k}, ~}{n}
\end{aligned}
$$



画 Carl De Boor．
On uniform approximation by splines．
J．Approx．Theory，1（1）：219－235， 1968.
囯 Charles J Stone．
Additive regression and other nonparametric models．
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