# NONPARAMETRIC ESTIMATION OF ADDITIVE MODELS 

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## INTRODUCTION

- Single-index model achieves dimension reduction by assuming that $\boldsymbol{E}(Y \mid X=x)=F\left(\beta^{\prime} X\right)$ for some unknown $F$ and $\beta$.
- Can estimate $\beta$ with $n^{-1 / 2}$ rate of convergence and $F$ with $n^{-2 / 5}$ rate if it is twice differentiable.
- A nonparametric additive model is alternative way to achieve dimension reduction.
- It has form

$$
\boldsymbol{E}(Y \mid X=x)=\mu+\sum_{j=1}^{d} m_{j}\left(x^{j}\right)
$$

where $\operatorname{dim}(X)=d, x^{j}$ is $j$ 'th component of $x$, and $\mu$ and the $m_{j}$ 's are unknown.

- Additive models are non-nested with single-index models
- A single-index model is not additive unless $F$ is the identity function.
- An additive model is not single-index unless the $m_{j}$ 's are linear.


## PROPERTIES OF ADDITIVE MODELS

- Additive components $m_{j}$ can be estimated with one-dimensional nonparametric rate of convergence ( $n^{-2 / 5}$ if the components are twice differentiable)
- Asymptotically normal estimators are available
- Each component can be estimated with same accuracy that it would have if other components were known
- This is called "oracle property."
- Three kinds of estimators are available:
- Marginal integration yields asymptotically normal estimators but is not oracle-efficient.
- Backfitting yields asymptotically normal, oracle efficient estimators.
- Two-step estimator based on seriesapproximation first step is asymptotically normal and oracle-efficient.


## MARGINAL INTEGRATION

- Model:

$$
\boldsymbol{E}(Y \mid X=x)=\mu+\sum_{j=1}^{d} m_{j}\left(x^{j}\right)
$$

- Need location normalization to identify the $m_{j}$ 's.
- Achieve this by setting $\boldsymbol{E}\left[m_{j}\left(X^{j}\right)\right]=0$.
- Get identifying relations
- $\mu=\boldsymbol{E}(Y)$

$$
m_{1}\left(x^{1}\right)=
$$

$$
\int \boldsymbol{E}\left(Y \mid X^{1}=x^{1}, X^{(-1)}=x^{(-1)}\right) p_{-1}\left(x^{(-1)}\right) d x^{(-1)}
$$

$-\mu$,
where $X^{(-1)}$ is vector consisting of all components of $X$ except $X^{1}$, and $p_{-1}$ is density of $X^{(-1)}$.

## ESTIMATION

- Estimate $\mu$ and $m_{1}$ by replacing population quantities with sample analogs in identifying relations
- This gives estimator of $\mu: \hat{\mu}=n^{-1} \sum_{i=1}^{n} Y_{i}$.
- Let $\hat{g}\left(x^{1}, x^{(-1)}\right)$ be nonparametric estimator of $\boldsymbol{E}\left(Y \mid X^{1}=x^{1}, X^{(-1)}=x^{(-1)}\right)$
- Example: Kernel or local linear estimator
- Estimator of $m_{1}$ is

$$
\hat{m}_{1}\left(x^{1}\right)=n^{-1} \sum_{i=1}^{n} \hat{g}\left(x^{1}, X_{i}^{(-1)}\right)-\hat{\mu} .
$$

- Under regularity conditions:

$$
n^{2 / 5}\left[\hat{m}_{1}\left(x^{1}\right)-m_{1}\left(x^{1}\right)\right] \rightarrow^{d} N\left[b_{1}\left(x^{1}\right), V_{1}\left(x^{1}\right)\right]
$$

for suitable $b_{1}$ and $V_{1}$

## ASYMPTOTIC DISTRIBUTION

- If $\hat{g}$ is local-linear estimator with bandwidth $h=c_{h} n^{-2 / 5}$ and kernel $K$ in $x^{1}$ direction and other conditions hold, then

$$
\begin{aligned}
& b_{1}\left(x^{1}\right)=0.5 c_{h}^{2} R_{K} m_{1}^{\prime \prime}\left(X^{1}\right) \\
& V_{1}\left(x^{1}\right)=c_{h}^{-1} v_{K} \int \operatorname{Var}\left(U \mid x^{1}, x^{(-1)}\right) \frac{p_{-1}^{2}\left(x^{(-1)}\right)}{p(x)} d x^{(-1)}
\end{aligned}
$$

where $p$ is density of $X$,

$$
\begin{aligned}
R_{K} & =\int v^{2} K(v) d v \\
v_{K} & =\int K(v)^{2} d v
\end{aligned}
$$

- In homoskedastic case

$$
V_{1}\left(x^{1}\right)=c_{h}^{-1} v_{K} \sigma_{U}^{2} \int \frac{p_{-1}^{2}\left(x^{(-1)}\right)}{p(x)} d x^{(-1)}
$$

- Oracle estimator gives $V_{1}\left(x^{1}\right)=c_{h}^{-1} v_{K} \sigma_{U}^{2} / p_{1}\left(x^{1}\right)$, which is smaller.
- Marginal integration estimator is not oracle efficient.


## PROPERTIES (cont.)

- Need $m_{j}$ 's and $p$ to have at least $d$ continuous derivatives
- So marginal integration estimator has curse of dimensionality
- This is caused by full-dimensional nonparametric estimation in first step.
- Marginal integration estimator is hard to compute.
- Computing $\hat{m}_{1}\left(x^{1}\right)$ requires $n$ nonparametric regressions for each value of $x^{1}$.
- Marginal integration estimator can be modified to overcome the curse of dimensionality.


## MODIFIED MI ESTIMATOR

- Write model as

$$
m(x)=\mu+m_{1}\left(x^{1}\right)+m_{-1}\left(x^{(-1)}\right)
$$

- Let $q_{1}$ and $q_{-1}$, respectively, be "smooth" density functions on $\mathbb{R}$ and $\mathbb{R}^{d-1}$, respectively.
- Define $q=q_{1} q_{-1}$
- Use location normalization
$\int m_{1}\left(x^{1}\right) q_{1}\left(x^{1}\right) d x^{1}=0$

$$
\int m_{-1}\left(x^{(-1)}\right) q_{-1}\left(x^{(-1)}\right) d x^{(-1)}=0
$$

- This normalization makes it possible to use smoothness of $q$ to reduce bias of estimator instead of using smoothness of $m$.


## ESTIMATOR (cont.)

- Let $h_{1}$ and $h_{2}$ be bandwidths, and $K$ and $L$ be kernel functions.
- Let $\hat{p}$ be kernel estimator of density of $X$.
- Define

$$
\begin{aligned}
& \tilde{m}_{n}(x)= \\
& \frac{1}{n h_{1} h_{2}^{d-1}} \sum_{i=1}^{n} \frac{Y_{i}}{\hat{p}\left(X_{i}\right)} K\left(\frac{x^{1}-X_{i}^{1}}{h_{1}}\right) L\left(\frac{x^{(-1)}-X_{i}^{(-1)}}{h_{2}}\right)
\end{aligned}
$$

This is form of kernel estimator of $\boldsymbol{E}(Y \mid X=x)$.

- Define

$$
\eta_{1}\left(x^{1}\right)=\int m(x) q_{-1}\left(x^{(-1)}\right) d x^{(-1)}-\mu .
$$

- Under location normalization $\eta_{1}=m_{1}$
- Estimator of $\eta_{1}$ is

$$
\begin{gathered}
\tilde{\eta}_{1}\left(x^{1}\right)=\int \tilde{m}_{n}(x) q_{-1}\left(x^{-1}\right) d x^{-1} \\
-\int \tilde{m}_{n}(x) q(x) d x
\end{gathered}
$$

## PROPERTIES

- Hengartner and Sperlich (2005) give conditions under which
$n^{2 / 5}\left[\hat{\eta}_{1}\left(x^{1}\right)-\eta_{1}\left(x^{1}\right)\right] \rightarrow^{d} N\left[b_{\eta 1}\left(x^{1}\right), V_{\eta}\left(x^{1}\right)\right]$
where $b_{h 1}$ and $V_{\eta}$ are the bias and variance functions.
- Conditions require $m$ to be only twice differentiable, regardless of $\operatorname{dim}(X)$.
- Therefore, curse of dimensionality is avoided
- But modified estimator is not oracle efficient.
- Computation can be simplified by letting $q_{-1}$ be Dirac $\delta$ function centered at some $x^{(-1)}$ value.
- This gives

$$
\tilde{\eta}\left(x^{1}\right)=\tilde{m}_{n}\left(x^{1}, x^{(-1)}\right)-\int \tilde{m}_{n}\left(z^{1}, x^{(-1)}\right) q_{1}\left(z^{1}\right) d z^{1}
$$

- Asymptotic normality and rate result still holds
- Hengartner and Sperlich do not investigate extent to which this causes loss of asymptotic efficiency


## ACHIEVING ORACLE EFFICIENCY

- Oracle efficiency means: Estimator of each additive component has asymptotic distribution it would have if the other components were known
- Asymptotically, there is no penalty for having to estimate other components.
- Marginal integration estimators are not oracle efficient but can be made so by taking one "backfitting" step.
- Main idea: Suppose $m_{2}, \ldots, m_{d}$ and $\mu$ were known.
- Define $W_{i}=Y_{i}-\mu-m_{2}\left(X_{i}^{2}\right)-\ldots-m_{d}\left(X_{i}^{d}\right)$
- Then model is

$$
W_{i}=m_{1}\left(X_{i}^{1}\right)+U_{i}
$$

- Can estimate $m_{1}$ by, for example, kernel or locallinear regression of $W$ on $X^{1}$
- Estimator is oracle efficient by definition.


## ACHIEVING ORACLE EFFICIENCY (cont.)

- In applications, replace $\mu, m_{2}, \ldots, m_{d}$ with preliminary (possibly marginal integration) estimates $\tilde{\mu}, \tilde{m}_{2}, \ldots, \tilde{m}_{d}$.
- Define $\tilde{W}_{i}=Y_{i}-\tilde{\mu}-\tilde{m}_{2}\left(X_{i}^{2}\right)-\ldots-\tilde{m}_{d}\left(X_{i}^{d}\right)$
- Estimate $m_{1}$ by kernel or local-linear regression of $\tilde{W}$ on $X^{1}$
- For case $d=2$, Linton (1997) gives conditions under which resulting estimator of $m_{1}$ is asymptotically normal with same mean and variance as estimator from regression of $W_{i}$ on $X_{i}^{1}$.
- Conditions include undersmoothing in estimating the $\tilde{m}_{j}$ 's $(j=2, \ldots, d)$.
- This makes the bias of preliminary estimator asymptotically negligible
- Variance increases but is reduced by the averaging entailed in second estimation step.
- Is unknown whether oracle efficiency for $d>2$ can be achieved by starting with Hengartner-Sperlich estimator


## ACHIEVING ORACLE EFFICIENCY (cont.)

- Other methods are available for achieving oracle efficiency with $d>2$
- Two-step estimation can be used in more general settings to achieve oracle efficiency.


## BACKFITTING

- For $j=1, \ldots, d$, define

$$
W_{j}=Y_{i}-\mu-\sum_{k \neq j} m_{k}\left(X_{i}^{k}\right)
$$

- Write model as

$$
W_{j}=m_{j}\left(X_{i}^{j}\right)+U_{i}
$$

- Let $\hat{\mu}^{0}, \hat{m}_{2}^{0}, \ldots, \hat{m}_{d}^{0}$ be preliminary estimates, and set

$$
\hat{W}_{1}^{0}=Y_{i}-\hat{\mu}^{0}-\sum_{j=2}^{d} \hat{m}_{j}^{0}\left(X_{i}^{j}\right)
$$

- Backfitting consists of:
- Estimate $m_{1}$ by nonparametric regression of $\hat{W}_{1}^{0}$ on $X^{1}$. Let $\hat{m}_{1}^{1}$ denote resulting estimate.
- $\operatorname{Set} \hat{W}_{2}^{1}=Y_{i}-\hat{\mu}^{0}-\hat{m}_{1}^{1}\left(X_{i}^{1}\right)-\sum_{j=3}^{d} \hat{m}_{j}^{0}\left(X_{i}^{j}\right)$
- Estimate $m_{2}$ by nonparametric regression of $\hat{W}_{2}^{1}$ on $X^{2}$. Let $\hat{m}_{2}^{1}$ denote resulting estimate.


## BACKFITTING (cont.)

- Set

$$
\hat{W}_{3}^{1}=Y_{i}-\hat{\mu}^{0}-\hat{m}_{1}^{1}\left(X_{i}^{1}\right)-\hat{m}_{2}^{1}\left(X_{i}^{2}\right)-\sum_{j=3}^{d} \hat{m}_{j}^{0}\left(X_{i}^{j}\right)
$$

- Iterate procedure to convergence, thus obtaining estimators of all additive components and $\mu$
- This version of backfitting is hard to analyze theoretically
- Little known about its convergence or distributional properties
- Modified versions of backfitting are easier to analyze
- Mammen et al. (1999) have found conditions under which a suitably modified version is asymptotically normal and oracle efficient


## MODIFIED BACKFITING

- Notation
- $\breve{m}_{j}\left(x^{j}\right)$ denotes Nadaraya-Watson kernel estimator of $\boldsymbol{E}\left(Y \mid X^{j}=x^{j}\right)$.
- $\hat{p}_{j}$ and $\hat{p}_{j k}$, respectively are kernel estimators of density of $X^{j}$ and joint density of $\left(X^{j}, X^{k}\right)$
- $\tilde{m}_{j}^{0}$ is initial guess at estimator of $m_{j}$, possibly $\breve{m}_{j}$ or a marginal integration estimator

$$
\hat{p}_{k,[j+]}\left(x^{k}\right)=\int \hat{p}_{j k}\left(x^{j}, x^{k}\right) d x^{j}\left[\int \hat{p}_{j}\left(x^{j}\right) d x^{j}\right]^{-1}
$$

$$
\tilde{m}_{0, j}=\frac{\int \hat{m}_{j}\left(x^{j}\right) \hat{p}_{j}\left(x^{j}\right) d x^{j}}{\int \hat{p}_{j}\left(x^{j}\right) d x^{j}}
$$

- Location normalization: $\operatorname{Em}_{j}\left(X^{j}\right)=0$.


## ITERATIVE SCHEME AND ASYMPTOTICS

- In $r$ 'th iteration, estimate of $m_{j}$ is

$$
\begin{aligned}
& \tilde{m}_{j}^{r}\left(x^{j}\right)=\breve{m}_{j}\left(x^{j}\right)-\tilde{m}_{0, j} \\
& -\sum_{k<j} \int \tilde{m}_{k}^{r}\left(x^{k}\right)\left[\frac{\hat{p}_{j k}\left(x^{j}, x^{k}\right)}{\hat{p}_{j}\left(x^{j}\right)}-\hat{p}_{k,[j+]}\left(x^{k}\right)\right] d x^{k} \\
& -\sum_{k>j} \int \tilde{m}_{k}^{[r-1]}\left(x^{k}\right)\left[\frac{\hat{p}_{j k}\left(x^{j}, x^{k}\right)}{\hat{p}_{j}\left(x^{j}\right)}-\hat{p}_{k,[j+]}\left(x^{k}\right)\right] d x^{k}
\end{aligned}
$$

- Mammen, Linton, and Nielsen show that if the $m_{j}$ 's are twice continuously differentiable and some other conditions are satisfied, then
- The iterative scheme converges to limiting estimators $\tilde{m}_{j}$
- $n^{1 / 2}\left[\tilde{m}_{j}-m_{j}\left(x^{j}\right)\right]$ are asymptotically normally distributed for any finite $d$ (no curse of dimensionality).
- The mean and variance of the asymptotic distribution are oracle


## COMMENTS ON BACKFITTING

- Modified backfitting estimator avoids curse of dimensionality and is oracle efficient but is analytically and computationally complicated
- Taking one backfitting step from HengartnerSperlich estimator may produce simpler oracleefficient estimator, but this is not yet proved.
- Next lecture will present approach that uses series estimation in first step followed by a backfitting step
- This method is simpler computationally than marginal integration or modified backfitting
- It is oracle efficient
- Can be applied to additive quantile regressions and models with link functions.


## EMPIRICAL EXAMPLE

- Use data from Current Population Survey to estimate wage function
$\boldsymbol{E}(\log W \mid E X P, E D U C)=$

$$
\mu+f_{E X P}(E X P)+f_{E D U C}(E D U C)
$$

- $E X P$ and $E D U C$ are years of experience and education.
- Population is white males with 14 or fewer years of education who work full time and live in urban areas in North Central U.S.




## COMMENTS ON ESTIMATION RESULTS

- Estimates of $f_{\text {EXP }}$ and $f_{\text {EDUC }}$ are nonlinear and differently shaped
- Functions $f_{\text {EXP }}$ and $f_{E D U C}$ with different shapes cannot be produced by a single-index model
- A lengthy specification search might be needed to find a parametric model that produces the shapes shown in the figure
- Some of the fluctuations of the estimates of $f_{E D U C}$ and $f_{\text {EDUC }}$ may be artifacts of random sampling errors.
- But a more elaborate analysis rejects the hypothesis that either function is linear.


## CONCLUSIONS

- Nonparametric additive model

$$
\boldsymbol{E}(Y \mid X=x)=\mu+\sum_{j=1}^{d} m_{j}\left(x^{j}\right)
$$

- Additive components $m_{j}$ can be estimated so as to:
- Achieve one-dimensional nonparametric rate of convergence (dimension reduction) \}
- Have asymptotical normal limiting distributions
- Achieve oracle efficiency

