# NONPARAMETRIC ESTIMATION OF AN ADDITIVE MODEL WITH A LINK FUNCTION 

by

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## INTRODUCTION

- Problem: Estimate $H(x)=E(Y \mid X=x)$ under weak assumptions about its functional form when $X$ is a continuous random variable
- Fully nonparametric estimation is unattractive when $X$ is multidimensional because of the curse of dimensionality.
- Dimension reduction methods reduce effective dimension of estimation problem and mitigate or eliminate curse of dimensionality
- They make assumptions about the form of $H(x)$ that are stronger than those of a fully nonparametric model but weaker than those of a parametric model


## DIMENSION REDUCTION METHODS

- Semiparametric single-index model
- Additive model with known link function

$$
H(x)=F\left[\mu+\sum_{j=1}^{d} m_{j}\left(x^{j}\right)\right]
$$

where $F$ is known, and $\mu$ and $m_{j}$ 's are unknown.

- Partially linear model with known link function (Robinson 1988, Golubev and Härdle 1997, Severini and Staniswalis 1994)

$$
E(Y \mid X=x, W=w)=G\left[\beta^{\prime} x+f_{w}(w)\right]
$$

where $G$ is known but $\beta$ and $f_{w}$ are not.

- Additive model with unknown link function

$$
H(x)=F\left[\sum_{j=1}^{d} m_{j}\left(x^{j}\right)\right]
$$

where $F$ and the $m_{j}$ 's are unknown.

## PURPOSE OF THIS PAPER

Paper is concerned with estimating nonparametric additive model with known link function.

- Marginal integration estimator (Linton and Härdle 1996) has curse-of-dimensionality
- Smoothness of the $m_{j}$ 's must increase as dimension of $X$ increases to achieve $n^{-2 / 5}$ rate of convergence of nonparametric estimator of the $m_{j}$ 's.
- If $F$ is identity function, this problem can be overcome by use of backfitting
- Methods for achieving $n^{-2 / 5}$ rate of convergence with no curse of dimensionality not available with non-identity $F$.
- This paper develops method for avoiding curse of dimensionality in estimating nonparametric additive model with known link function.
- Estimator is pointwise $n^{2 / 5}$-consistent and asymptotically normal when $F$ and the $m_{j}$ 's are twice differentiable, regardless of dimension of $X$.


## MARGINAL INTEGRATION ESTIMATOR (Linton and Härdle 1996)

- Define $G=F^{-1}$ and $H(x)=\boldsymbol{E}(Y \mid X=x)$.
- Linton and Härdle (1996) write model in form
$G\left[H\left(x^{1}, \ldots, x^{d}\right)\right]=\mu+m_{1}\left(x^{1}\right)+\ldots+m_{d}\left(x^{d}\right)$,
where $G=F^{-1}$ and $\boldsymbol{E}\left[m_{j}\left(X^{j}\right)\right]=0$.
- Therefore
$\mu+m_{1}\left(x^{1}\right)=\boldsymbol{E} G\left[H\left(x^{1}, X^{2}, \ldots, X^{d}\right)\right]$.
- Estimate $m_{1}\left(x^{1}\right)$ up to additive constant by replacing $H$ with kernel estimator and $\boldsymbol{E}$ with sample average.
- This creates curse-of-dimensionality effect because a $d$-dimensional nonparametric regression is needed to estimate $H$.
- More smoothness needed as $d$ increases to insure bias and variance of full-dimensional estimator are sufficiently small.


## SOLUTION TO PROBLEM

- Avoid curse of dimensionality by replacing kernel estimator with estimator that does not require fulldimensional nonparametric regression.
- Nonparametric series approximation can be used to impose additive structure from outset, thereby avoiding need for full-dimensional estimation.
- Getting pointwise rates of convergence and asymptotic normality with series estimator is difficult
- Use two-step procedure to obtain estimator with tractable asymptotics:
- Step 1: Use nonparametric series estimation to obtain pilot estimates $\tilde{\mu}, \tilde{m}_{1}, \ldots, \tilde{m}_{d}$
- Step 2: Take one Newton step from pilot estimates toward local constant or local linear least squares estimator of (say) $m_{1}$
- Second-stage estimator has structure of kernel estimator, so its asymptotic distribution can be obtained easily.


## FURTHER MOTIVATION

- If $\mu$ and $m_{2}, \ldots, m_{d}$ were known, could estimate $m_{1}\left(x^{1}\right)$ by (say) local nonlinear least squares:

$$
\begin{aligned}
& \hat{m}_{1}\left(x^{1}\right)=\arg \min _{m_{1}} \sum_{i=1}^{n}\left\{Y_{i}-F\left[\mu+m_{1}\left(x^{1}\right)\right.\right. \\
& \left.\left.\quad+m_{2}\left(X_{i}^{2}\right)+\ldots+m_{d}\left(X_{i}^{d}\right)\right]\right\}^{2} K_{h}\left(x^{1}-X_{i}^{1}\right)
\end{aligned}
$$

where $K_{h}\left(x^{1}-X_{i}^{1}\right)=K\left[\left(x^{1}-X_{i}^{1}\right) / h\right], K$ is kernel.

- Replace unknown $\mu$ and $m_{2}, \ldots, m_{d}$ with pilot estimates to get kernel-like estimator of $m_{1}\left(x^{1}\right)$.
- Undersmooth pilot estimates to reduce bias
- Resulting $\hat{m}_{1}\left(x^{1}\right)$ is asymptotically equivalent to estimator that would be obtained if $\mu$ and $m_{2}, \ldots, m_{d}$ were known.
- So there is (asymptotically) no penalty for not knowing $\mu$ and $m_{2}, \ldots, m_{d}$ and no curse of dimensionality.


## AVOIDING NONLINEAR OPTIMIZATION

- Nonparametric series estimation yields estimate $\tilde{m}_{1}$ of $m_{1}$.
- Avoid nonlinear optimization by taking one Newton step from pilot estimate toward solution of local least squares problem.
- Resulting estimator is asymptotically equivalent to solution of full nonlinear optimization.
- Define $\tilde{m}_{-1}\left(x_{-1}\right)=\tilde{m}_{2}\left(x^{2}\right)+\ldots+\tilde{m}_{d}\left(x^{d}\right)$,
$S_{n 1}\left(x^{1}, \tilde{m}\right)=$

$$
\sum_{i=1}^{n}\left\{Y_{i}-F\left[\tilde{\mu}+\tilde{m}_{1}\left(x^{1}\right)+\tilde{m}_{-1}\left(\tilde{X}_{i}\right)\right]\right\}^{2} K_{h}\left(x^{1}-X_{i}^{1}\right)
$$

$S_{n 1}{ }^{\prime}\left(x^{1}, \tilde{m}\right), S_{n 1}{ }^{\prime \prime}\left(x^{1}, \tilde{m}\right)$ are first and second derivatives of $S_{n 1}$ with respect to $\tilde{m}_{1}$

## SECOND-STAGE ESTIMATOR

- Second-stage estimator is

$$
\hat{m}_{1}\left(x^{1}\right)=\tilde{m}_{1}\left(x^{1}\right)-S_{n 1}^{\prime}\left(x^{1}, \tilde{m}\right) / S_{n 1}^{\prime \prime}\left(x^{1}, \tilde{m}\right) .
$$

## NONPARAMETRIC SERIES ESTIMATOR

- Define $m(x)=m_{1}\left(x^{1}\right)+\ldots+m_{d}\left(x^{d}\right)$
- Let support of $X$ be $[-1,1]^{d}$.
- Normalize $m_{j}$ 's by $\int_{-1}^{1} m_{j}(v) d v=0(j=1, \ldots, d)$.
- Let $\left\{p_{k}: k=1,2, \ldots\right\}$ denote basis for smooth functions on $[-1,1]$ that satisfy normalization condition and

$$
\begin{aligned}
& \int_{-1}^{1} p_{k}(v) d v=0 \\
& \int_{-1}^{1} p_{j}(v) p_{k}(v) d v= \begin{cases}1 & \text { if } j=k \\
0 & \text { otherwise }\end{cases} \\
& m_{j}\left(x^{j}\right)=\sum_{k=1}^{\infty} \theta_{j k} p_{k}\left(x^{j}\right) ; \quad j=1, \ldots, d ; x^{j} \in[0,1]
\end{aligned}
$$

- For any positive integer $\kappa>0$ define

$$
P_{\kappa}(x)=\left[1, p_{1}\left(x^{1}\right), \ldots, p_{\kappa}\left(x^{1}\right), \ldots, p_{1}\left(x^{d}\right), \ldots, p_{\kappa}\left(x^{d}\right)\right]^{\prime}
$$

- Then for $\theta_{\kappa} \in \mathbb{R}^{\kappa d+1}, \quad P_{\kappa}(x)^{\prime} \theta_{\kappa} \quad$ is series approximation to $\mu+m(x)$.


## FIRST-STEP ESTIMATOR

- Let $\left\{Y_{i}, X_{i}: i=1, \ldots, n\right\}$ be random sample of $(Y, X)$
- Let $\hat{\theta}_{n \kappa}$ be solution to
$\underset{\theta \in \Theta_{\kappa}}{\operatorname{minimize}}: n^{-1} \sum_{i=1}^{n}\left\{Y_{i}-F\left[P_{\kappa}\left(X_{i}\right)^{\prime} \theta\right]\right\}^{2}$
where $\Theta_{\kappa}$ is compact parameter set.
- Series estimator of $\mu+m(x)$ is

$$
\tilde{\mu}+\tilde{m}(x)=P_{\kappa}(x)^{\prime} \hat{\theta}_{n \kappa},
$$

where $\tilde{\mu}$ is first component of $\hat{\theta}_{n \kappa}$.

- First-step estimator of $m_{j}\left(x^{j}\right)$ is product of [ $\left.p_{1}\left(x^{j}\right), \ldots, p_{\kappa}\left(x^{j}\right)\right]$ with appropriate subvector of $\hat{\theta}_{n \kappa}$.


## ASSUMPTIONS

- Data are random sample of $(Y, X)$, support of $X$ is $\mathcal{X} \equiv[-1,1]^{d}$, and $\boldsymbol{E}(Y \mid X=x)=F[\mu+m(x)]$.
- Density of $X$ is bounded, bounded away from zero, and twice differentiable.
- Set $U \equiv Y-F[\mu+m(X)]$. Then:
- $\operatorname{Var}(U \mid X=x)$ is bounded and bounded away from zero.
- $U$ has finite unconditional moments of all orders
- The $m_{j}$ 's are bounded and twice continuously differentiable

Only two derivatives needed regardless of dimension of $X$.

- $F^{\prime \prime}$ satisfies Lipschitz condition
$\left|F^{\prime \prime}\left(v_{2}\right)-F^{\prime \prime}\left(v_{1}\right)\right| \leq C\left|v_{2}-v_{1}\right|^{s}$
for some $s>5 / 7$.
- Conditions insuring that covariance matrix of $\hat{\theta}_{n \kappa}$ 's is bounded and non-singular.


## MORE ASSUMPTIONS

- Basis functions satisfy
$\sup \left\|P_{\kappa}(x)\right\|=O\left(\kappa^{1 / 2}\right)$
$x \in \mathcal{X}$
$\sup \left|\mu+m(x)-P_{\kappa}(x)^{\prime} \theta_{\kappa 0}\right|=O\left(\kappa^{-2}\right)$
$x \in \mathcal{X}$
for some $\theta_{\kappa 0} \in \Theta_{\kappa}$
These conditions are satisfied by spline and (for periodic functions) Fourier bases.
- Smoothing parameters satisfy:
- $\kappa=C_{\kappa} n^{4 / 15+v}$ for some $v<1 / 30$
- $h_{n}=C_{h} n^{-1 / 5}$

The $L_{2}$ rate of convergence of series estimator is maximized by setting $\kappa \propto n^{1 / 5}$, so the series estimator here is undersmoothed to reduce asymptotic bias.

- Kernel function $K$ of second-stage estimator is a bounded, continuous probability density function on $[-1,1]$ and is symmetrical about 0 .


## MAIN RESULTS: FIRST-STAGE ESTIMATOR

- Uniform consistency:

$$
\sup _{x \in \mathcal{X}}|\tilde{m}(x)-m(x)|=O_{p}\left(\kappa / n^{1 / 2}+\kappa^{-3 / 2}\right)
$$

- Decomposition: Define

$$
Q_{\kappa}=\boldsymbol{E}\left\{F^{\prime}[\mu+m(X)]^{2} P_{\kappa}(X) P_{\kappa}(X)^{\prime}\right\}
$$

Then

$$
\begin{aligned}
& \hat{\theta}_{n \kappa}-\theta_{\kappa 0}=n^{-1} Q_{\kappa}^{-1} \sum_{i=1}^{n} F^{\prime}\left[\mu+m\left(X_{i}\right)\right] P_{\kappa}\left(X_{i}\right) U_{i} \\
& \quad+n^{-1} Q_{\kappa}^{-1} \sum_{i=1}^{n} F^{\prime}\left[\mu+m\left(X_{i}\right)\right]^{2} P_{\kappa}\left(X_{i}\right) b_{\kappa}\left(X_{i}\right)+R_{n}
\end{aligned}
$$

$$
\text { where }\left\|R_{n}\right\|=O_{p}\left(\kappa^{3 / 2} / n+n^{-1 / 2}\right)
$$

## MAIN RESULTS: SECOND-STAGE ESTIMATOR

- Asymptotic representation: Define

$$
D\left(x^{1}\right)=\operatorname{plim}_{n \rightarrow \infty} S_{n 1}^{\prime \prime}\left(x^{1}, \tilde{m}\right)
$$

Then

$$
\begin{aligned}
& \left(n h_{n}\right)^{1 / 2}\left[\hat{m}_{1}\left(x^{1}\right)-m_{1}\left(x^{1}\right)\right]= \\
& \quad-\left(n h_{n}\right)^{1 / 2} S_{n 1}^{\prime}\left(x^{1}, m\right) / D\left(x^{1}\right)+o_{p}(1)
\end{aligned}
$$

This is representation that would be obtained by linearizing first-order condition for local leastsquares estimation of $m_{1}$ with known $m_{2}, \ldots, m_{d}$.
So asymptotically there is no penalty for not knowing $m_{2}, \ldots, m_{d}$.

Structure of right-hand side is same as with kernel estimator.

## RESULTS (cont.)

- Asymptotic normality

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

This holds when the $m_{j}$ 's are twice continuously differentiable, regardless of dimension of $X$.

So there is no curse of dimensionality.

- If $j \neq 1$, then $n^{2 / 5}\left[\hat{m}_{1}\left(x^{1}\right)-m_{1}\left(x^{1}\right)\right] \quad$ and $n^{2 / 5}\left[\hat{m}_{j}\left(x^{j}\right)-m_{j}\left(x^{j}\right)\right] \quad$ are asymptotically independently normally distributed.


## INTUITION FOR SECOND-STAGE RESULT

- Second-stage estimator is

$$
\hat{m}_{1}\left(x^{1}\right)=\tilde{m}_{1}\left(x^{1}\right)-S_{n 1}^{\prime}\left(x^{1}, \tilde{m}\right) / S_{n 1}^{\prime \prime}\left(x^{1}, \tilde{m}\right)
$$

- This can be written:

$$
\begin{aligned}
& \left(n h_{n}\right)^{1 / 2}\left[\hat{m}_{1}\left(x^{1}\right)-m_{1}\left(x^{1}\right)\right]= \\
& \quad=\left(n h_{n}\right)^{1 / 2}\left[\tilde{m}_{1}\left(x^{1}\right)-m_{1}\left(x^{1}\right)\right] \\
& \quad-\left(n h_{n}\right)^{1 / 2} S_{n 1}^{\prime}\left(x^{1}, \tilde{m}\right) / D\left(x^{1}\right)+o_{p}(1)
\end{aligned}
$$

- Use Taylor series approximation to write

$$
\left(n h_{n}\right)^{1 / 2} S_{n 1}^{\prime}\left(x^{1}, \tilde{m}\right)=
$$

$$
\left(n h_{n}\right)^{1 / 2} S_{n 1}^{\prime}\left(x^{1}, m\right)+T_{n 1}+T_{n 2}+o_{p}(1)
$$

## INTUITION (cont.)

- $T_{n 1}=D\left(x^{1}\right)\left(n h_{n}\right)^{1 / 2}\left[\tilde{m}_{1}\left(x^{1}\right)-m_{1}\left(x^{1}\right)\right]+o_{p}(1)$
- So
$\left(n h_{n}\right)^{1 / 2}\left[\hat{m}_{1}\left(x^{1}\right)-m_{1}\left(x^{1}\right)\right]=$

$$
-\left(n h_{n}\right)^{1 / 2} S_{n 1}^{\prime}\left(x^{1}, m\right) / D\left(x^{1}\right)+T_{n 2}+o_{p}(1)
$$

- $T_{n 2}$ consists of
- Bias term arising from asymptotic bias of $\tilde{m}_{1}$
- Sum of mean-zero stochastic terms arising from random component of $\hat{\theta}_{n \kappa}-\theta_{\kappa 0}$
- Because first-stage estimator is undersmoothed

$$
\left(n h_{n}\right)^{1 / 2}[\text { Bias Term }]=o_{p}(1)
$$

- Contribution of bias term to $T_{n 2}$ is asymptotically negligible.


## INTUITION (cont.)

- Stochastic terms have slower than $n^{-2 / 5}$ rates of convergence but are averaged in $T_{n 2}$.
- First-stage estimator has no curse of dimensionality, so rate of convergence of variance of stochastic term does not increase with increasing dimension of $X$.
- Averaged stochastic term converges faster than $n^{-2 / 5}$.
- So contribution of stochastic term to $T_{n 2}$ is negligible.
- Consequently, $T_{n 2}$ is asymptotically negligible.


## BANDWIDTH SELECTION

- Asymptotic integrated mean-square error of $\hat{m}_{1}$ is
$A I M S E_{1}=n^{4 / 5} \int_{-1}^{1} w\left(x^{1}\right)\left[\beta_{1}\left(x^{1}\right)^{2}+V_{1}\left(x^{1}\right)\right] d x^{1}$,
where $w$ is a weight function.
- $A I M S E_{1}$ minimized by setting $h=C_{h 1} n^{-1 / 5}$, where

$$
\begin{aligned}
& C_{h 1}=\left[(1 / 4) \frac{\int_{-1}^{1} w\left(x^{1}\right) \tilde{V}_{1}\left(x^{1}\right) d x^{1}}{\int_{-1}^{1} w\left(x^{1}\right) \tilde{\beta}_{1}\left(x^{1}\right)^{2} d x^{1}}\right]^{1 / 5}, \\
& \tilde{\beta}_{1}\left(x^{1}\right)=\beta_{1}\left(x^{1}\right) / C_{h}^{2} \text { and } \tilde{V}_{1}\left(x^{1}\right)=C_{h} V_{1}\left(x^{1}\right) .
\end{aligned}
$$

- Plug-in estimator of $C_{h 1}$ can be obtained by replacing $\tilde{\beta}_{1}$ and $\tilde{V}_{1}$ with kernel estimates.
- The asymptotically optimal bandwidths for all the $m_{j}$ 's can be estimated simultaneously by penalized least squares.
- This minimizes empirical analog of asymptotic squared error:


## MONTE CARLO EXPERIMENTS

- Compare finite-sample performance of new estimator with that of Linton and Härdle (1996)
- New estimator implemented using local constant and local linear smoothing in second stage.
- Experiments carried out with $d=2$ and $d=5$.
- L-H estimator is $O_{p}\left(n^{-2 / 5}\right)$ if $d=2$, not $d=5$.
- Sample size is $n=500$
- With $d=2$ estimate $m_{1}$ and $m_{2}$ in logit model
- $\boldsymbol{P}(Y=1 \mid X=x)=L\left[m_{1}\left(x^{1}\right)+m_{2}\left(x^{2}\right)\right]$
- $L(v)=e^{v} /\left(1+e^{v}\right)$
- $m_{1}\left(x^{1}\right)=\sin \left(\pi x^{1}\right)$
- $m_{2}\left(x^{2}\right)=\Phi\left(3 x^{2}\right)$, where $\Phi$ is normal CDF
- With $d=5$ estimate $m_{1}$ and $m_{2}$ in logit model

$$
\boldsymbol{P}(Y=1 \mid X=x)=L\left[m_{1}\left(x^{1}\right)+m_{2}\left(x^{2}\right)+\sum_{j=3}^{5} x^{j}\right]
$$

- Components of $X$ are independently $U[-1,1]$.


## MONTE CARLO EXPERIMENTS (cont.)

- B-splines used for first-stage series estimator
- Second-order kernel used for second-stage estimator
- Tuning parameters chosen to minimize empirical integrated mean-square errors.
- 1000 replications with 2 -stage estimator but only 500 with Linton-Härdle estimator


## RESULTS

|  | Empirical IMSE |  |  |
| :---: | :---: | :---: | :---: |
| Estimator | $f_{1}$ | $f_{2}$ |  |
|  | $d=2$ |  |  |
| FHS |  | .116 | .015 |
| 2-Stage LC |  | .052 | .015 |
| 2-Stage LL |  | .052 | .023 |
|  | $d=5$ |  |  |
| FHS |  | .145 | .019 |
| 2-Stage LC | .060 | .018 |  |
| 2-Stage LL | .057 | .029 |  |

- Local constant and local linear estimators both dominate Linton-Härdle for estimating $f_{1}$
- For estimating $f_{2}$ Local constant and LintonHärdle estimators have roughly same IMSE
- Local linear estimator is worse


## CONCLUSIONS

- Paper has considered additive model with known link function
$\boldsymbol{E}(Y \mid X=x)=F\left[\mu+m^{1}\left(x^{1}\right)+\ldots+m_{j}\left(x^{j}\right)\right]$
- Marginal integration estimator of Linton and Härdle (1996) has curse of dimensionality
- Backfitting method of Mammen et al. (1999) avoids curse of dimensionality if $F$ is identity function
- This paper has proposed two-step method for avoiding curse of dimensionality with non-identity link function.
- First step uses nonparametric series estimator that imposes additive structure
- Second step takes a Newton step from series estimate toward a local least squares estimator.
- Second-stage estimator has structure of kernel estimator and is pointwise asymptotically normal with $n^{-2 / 5}$ rate of convergence regardless of dimension of $X$.

