

A note on the backfitting estimation of additive models

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The additive model is one of the most popular semi-parametric models. The backfitting estimation (Buja, Hastie and Tibshirani, *Ann. Statist.* **17** (1989) 453–555) for the model is intuitively easy to understand and theoretically most efficient (Opsomer and Ruppert, *Ann. Statist.* **25** (1997) 186–211); its implementation is equivalent to solving simple linear equations. However, convergence of the algorithm is very difficult to investigate and is still unsolved. For bivariate additive models, Opsomer and Ruppert (*Ann. Statist.* **25** (1997) 186–211) proved the convergence under a very strong condition and conjectured that a much weaker condition is sufficient. In this short note, we show that a weak condition can guarantee the convergence of the backfitting estimation algorithm when Nadaraya–Watson kernel smoothing is used.

Keywords: additive model; backfitting algorithm; convergence of algorithm; kernel smoothing

1. Introduction

The additive model has been proven to be a very useful semi-parametric model and is popularly used in practice. An intuitive implementation of the estimation is the backfitting approach (Buja, Hastie and Tibshirani (1989), called BHT hereafter). It is noticed that the implementation can be done easily by solving linear normal equations (page 476, BHT) *if the backfitting algorithm converges*. However, to justify the convergence of the algorithm is not easy. BHT provided sufficient conditions that guarantee the convergence of the backfitting algorithm or, equivalently, the existence of the estimators. These conditions are only generally satisfied by regression splines and other methods, but not by kernel smoothing. Some other approaches (e.g., Tjøstheim and Auestad (1994); Linton and Nielsen (1995); Mammen, Linton and Nielsen (1999); Wang and Yang (2007)) have been proposed to avoid difficult problems involving the convergence of the algorithm and the asymptotics of estimators. However, the original backfitting of BHT is still one of the most intuitive approaches.

Opsomer and Ruppert (1997), called OR hereafter, investigated the algorithm's convergence for the local polynomial kernel smoothing when the predictors are bivariate. Suppose that Y is the response and (U, V) are the bivariate predictor satisfying the additive model

$$Y = \alpha + m_1(U) + m_2(V) + \varepsilon, \quad (1)$$

where $E(\varepsilon|U, V) = 0$ almost surely. Constraints $E\{m_1(U)\} = E\{m_2(V)\} = 0$ are usually imposed for model identification; see, for example, OR. It is known (see, e.g., BHT) that the terms

in the model are the solution to minimizing

$$\min_{\substack{m_1 \in L_2, m_2 \in L_2, \\ \alpha \in R}} E\{Y - \alpha - m_1(U) - m_2(V)\}^2, \tag{2}$$

where L_2 is the measurable functional space with finite second moments. Let $f(u, v)$, $f_1(u)$ and $f_2(v)$ be the joint density function and marginal density functions of (U, V) , U and V respectively. OR required that

$$\sup_{u, v} \left| \frac{f(u, v)}{f_1(u)f_2(v)} - 1 \right| < 1$$

to prove the convergence of the backfitting algorithm. This requirement is very stringent and even excludes a significant amount of normal distributions. However, OR conjectured that the algorithm convergence can be guaranteed under very weak conditions. Next, we shall prove that their conjecture is correct when the Nadaraya–Watson kernel is used.

2. Main results

Suppose $\{(Y_i, U_i, V_i) : i = 1, \dots, n\}$ is a random sample from model (1). Following BHT, let $\mathbf{m}_1 = (m_1(U_1), \dots, m_1(U_n))^T$, $\mathbf{m}_2 = (m_2(V_1), \dots, m_2(V_n))^T$ and $\mathbf{Y} = (Y_1, \dots, Y_n)^T$. The estimators of functions m_1 and m_2 are determined by the estimation of function values at the observed points, that is, \mathbf{m}_1 and \mathbf{m}_2 . Let $K(\cdot) \geq 0$ be a kernel function and $K_h(\cdot) = K(\cdot/h)/h$ for any $h > 0$.

For the estimation of function values at U_i and V_i , we use (varying) bandwidths $h_i > 0$ and $\tilde{h}_i > 0$ respectively and kernel weights $\ell_i = [K_{h_i}(U_i - U_1), \dots, K_{h_i}(U_i - U_n)]^T / \sum_{k=1}^n K_{h_i} \times (U_i - U_k)$ and $\omega_i = [K_{\tilde{h}_i}(V_i - V_1), \dots, K_{\tilde{h}_i}(V_i - V_n)]^T / \sum_{k=1}^n K_{\tilde{h}_i}(V_i - V_k)$. Let

$$\mathbf{S}_1 = \begin{pmatrix} \ell_1^T \\ \vdots \\ \ell_n^T \end{pmatrix}, \quad \mathbf{S}_2 = \begin{pmatrix} \omega_1^T \\ \vdots \\ \omega_n^T \end{pmatrix}.$$

Corresponding to constraints $E\{m_1(U)\} = E\{m_2(V)\} = 0$, we introduce $(\mathbf{I}_n - \mathbf{1}_n \mathbf{1}_n^T/n)$, where \mathbf{I}_n is the $n \times n$ identity matrix and $\mathbf{1}_n$ is the $n \times 1$ vector with all entries 1. Let $\mathbf{S}_1^* = (\mathbf{I}_n - \mathbf{1}_n \mathbf{1}_n^T/n) \mathbf{S}_1$ and $\mathbf{S}_2^* = (\mathbf{I}_n - \mathbf{1}_n \mathbf{1}_n^T/n) \mathbf{S}_2$. Using kernel smoothing, the backfitting estimation procedure is iteratively

$$\hat{\mathbf{m}}_1^{\text{new}} := \mathbf{S}_1^* \{\mathbf{Y} - \hat{\mathbf{m}}_2^{\text{old}}\}, \quad \hat{\mathbf{m}}_2^{\text{new}} := \mathbf{S}_2^* \{\mathbf{Y} - \hat{\mathbf{m}}_1^{\text{old}}\}.$$

As BHT pointed out, the final estimators $\hat{\mathbf{m}}_1$ and $\hat{\mathbf{m}}_2$ of the algorithm are equivalent to the solution of

$$\begin{pmatrix} \mathbf{I}_n & \mathbf{S}_1^* \\ \mathbf{S}_2^* & \mathbf{I}_n \end{pmatrix} \begin{pmatrix} \hat{\mathbf{m}}_1 \\ \hat{\mathbf{m}}_2 \end{pmatrix} = \begin{pmatrix} \mathbf{S}_1^* \\ \mathbf{S}_2^* \end{pmatrix} \mathbf{Y}.$$

The solution exists if the inverse of $(\mathbf{I}_n - \mathbf{S}_2^* \mathbf{S}_1^*)$ or $(\mathbf{I}_n - \mathbf{S}_1^* \mathbf{S}_2^*)$ exists. If the iteration converges, then estimators of α , $\hat{\mathbf{m}}_1$ and $\hat{\mathbf{m}}_2$ are respectively $\hat{\alpha} = \bar{Y}$,

$$\hat{\mathbf{m}}_1 = \mathbf{S}_1^* (\mathbf{I}_n - \mathbf{S}_2^* \mathbf{S}_1^*)^{-1} (\mathbf{I}_n - \mathbf{S}_2^*) \mathbf{Y}$$

and

$$\hat{\mathbf{m}}_2 = (\mathbf{I}_n - \mathbf{S}_2^* \mathbf{S}_1^*)^{-1} \mathbf{S}_2^* (\mathbf{I}_n - \mathbf{S}_1^*) \mathbf{Y}$$

(the solutions can be rewritten in different forms). As we can see, the backfitting estimation is very easy to implement and is equivalent to a one-step calculation, if it converges. Thus, convergence of the algorithm is essential for the estimation of the additive model.

Theorem 1. Denote the order statistics of $\{U_1, \dots, U_n\}$ and $\{V_1, \dots, V_n\}$ by $\{U_{[1]}, \dots, U_{[n]}\}$ and $\{V_{[1]}, \dots, V_{[n]}\}$, respectively, and their corresponding bandwidths by $\{h_{[1]}, \dots, h_{[n]}\}$ and $\{\bar{h}_{[1]}, \dots, \bar{h}_{[n]}\}$, respectively. If kernel function $K(\cdot)$ and the bandwidths satisfy $K(0) > 0$,

$$\begin{aligned} K_{h_{[i]}}(U_{[i]} - U_{[i-1]}) > 0, & \quad K_{h_{[i]}}(U_{[i]} - U_{[i+1]}) > 0, \\ K_{\bar{h}_{[i]}}(V_{[i]} - V_{[i-1]}) > 0, & \quad K_{\bar{h}_{[i]}}(V_{[i]} - V_{[i+1]}) > 0 \end{aligned} \tag{3}$$

for $1 < i < n$, and

$$\begin{aligned} K_{h_{[1]}}(U_{[1]} - U_{[2]}) > 0, & \quad K_{h_{[n]}}(U_{[n]} - U_{[n-1]}) > 0, \\ K_{\bar{h}_{[1]}}(V_{[1]} - V_{[2]}) > 0, & \quad K_{\bar{h}_{[n]}}(V_{[n]} - V_{[n-1]}) > 0, \end{aligned} \tag{4}$$

then the backfitting algorithm converges.

Remark 1. Suppose that $K(\cdot)$ is a symmetric kernel function with $K(v) > 0$ for all $|v| < 1$ and that global (constant) bandwidths h and \bar{h} are used. If h and \bar{h} are greater than the largest difference between any two nearest points respectively, that is,

$$\begin{aligned} h &> \max\{U_{[i+1]} - U_{[i]}, i = 1, \dots, n - 1\} \quad \text{and} \\ \bar{h} &> \max\{V_{[i+1]} - V_{[i]}, i = 1, \dots, n - 1\}, \end{aligned} \tag{5}$$

then (3) and (4) hold. By Theorem 1, the convergence of the algorithm is guaranteed.

Corollary 1. Suppose U and V are distributed on compact intervals with density functions bounded away from 0. If global (constant) bandwidths h and \bar{h} are used with $h, \bar{h} \rightarrow 0$ and $nh / \log(n), n\bar{h} / \log(n) \rightarrow \infty$, then the algorithm converges in probability for n sufficiently large.

Remark 2. It is remarkable that the range of bandwidths for the algorithm to converge is quite wide, and that bandwidths $h \propto n^{-\delta}$ and $\bar{h} \propto n^{-\delta}$ with $0 < \delta < 1$ satisfy the requirement in Corollary 1. Thus, the algorithm converges. These bandwidths include the optimal bandwidths where $\delta = 1/5$ (see, e.g., OR).

This short note only considers the bivariate case with Nadaraya–Watson kernel smoothing. We conjecture that the backfitting estimation still converges under weak conditions for general additive models and other kernel estimation methods, including local polynomial smoothing. After the convergence is justified, asymptotics of the estimators can be obtained following exactly the same arguments as Opsomer and Ruppert (1997). The details are omitted.

3. Proofs

The proof of Theorem 1 is based on the properties of the regular Markov chain and the Perron–Frobenius theorem (see, e.g., Minc (1988)). The proof of Corollary 1 is based on the properties of order statistics (see, e.g., David and Nagaraja (2003)).

Proof of Theorem 1. We first prove that the absolute eigenvalues of \mathbf{S}_1 are all smaller than 1, with only one exception that equals 1. It is easy to see that \mathbf{S}_1 is a probability transition matrix of the Markov chain. By conditions (3) and (4), \mathbf{S}_1 is irreducible and aperiodic. Therefore, it is a regular transition probability matrix. There is an integer k such that all entries in \mathbf{S}_1^k are strictly positive (see, e.g., Romanovsky (1970), Theorem 14.I). By the Perron–Frobenius theorem, there is one (and only one) eigenvalue λ_1 of multiplicity 1 such that all entries in its corresponding eigenvector are positive. It is easy to see that this eigenvalue is $\lambda_1 = 1$ and its eigenvector is $\theta = \mathbf{1}_n/\sqrt{n}$, because the sum of any row in \mathbf{S}_1 is 1. Let $\lambda_2, \dots, \lambda_n$ be the other $n - 1$ eigenvalues of \mathbf{S}_1 (repeated eigenvalues are counted repeatedly). The Perron–Frobenius theorem also indicates that $1 = \lambda_1 > \max\{|\lambda_2|, \dots, |\lambda_n|\}$.

Next, we show that the absolute eigenvalues of $\mathbf{S}_1^* = (\mathbf{I}_n - \theta\theta^\top)\mathbf{S}_1$ are all strictly smaller than 1. Suppose that the eigenvalues $\lambda_2, \dots, \lambda_n$ of \mathbf{S}_1 are distinct and their corresponding eigenvectors are β_2, \dots, β_n , respectively (the general argument is similar, but needs more complicated notation). It is easy to check that θ and $(\mathbf{I}_n - \theta\theta^\top)\beta_k, k = 2, \dots, n$ are the eigenvectors of \mathbf{S}_1^* with corresponding eigenvalues being 0 and $\lambda_2, \dots, \lambda_n$, respectively, because

$$(\mathbf{I}_n - \theta\theta^\top)\mathbf{S}_1\theta = (\mathbf{I}_n - \theta\theta^\top)\lambda_1\theta = 0$$

and

$$\begin{aligned} (\mathbf{I}_n - \theta\theta^\top)\mathbf{S}_1(\mathbf{I}_n - \theta\theta^\top)\beta_k &= (\mathbf{I}_n - \theta\theta^\top)\{\mathbf{S}_1\beta_k - \mathbf{S}_1\theta\theta^\top\beta_k\} \\ &= (\mathbf{I}_n - \theta\theta^\top)\{\lambda_k\beta_k - \lambda_1\theta\theta^\top\beta_k\} \\ &= \lambda_k(\mathbf{I}_n - \theta\theta^\top)\beta_k - \lambda_1(\mathbf{I}_n - \theta\theta^\top)\theta\theta^\top\beta_k \\ &= \lambda_k(\mathbf{I}_n - \theta\theta^\top)\beta_k \quad \text{for } k = 2, \dots, n. \end{aligned}$$

Since the absolute values of $0, \lambda_2, \dots, \lambda_n$ are all smaller than 1, we have proven that the absolute eigenvalues of \mathbf{S}_1^* are smaller than 1. Applying the same argument to \mathbf{S}_2^* , we have that the absolute values of all eigenvalues of \mathbf{S}_2^* are smaller than 1.

Since the largest absolute eigenvalues of both \mathbf{S}_1^* and \mathbf{S}_2^* are smaller than 1, the absolute values of all eigenvalues of $\mathbf{S}_2^*\mathbf{S}_1^*$ and $\mathbf{S}_1^*\mathbf{S}_2^*$ are also smaller than 1. It follows that the inverses of $(\mathbf{I}_n - \mathbf{S}_2^*\mathbf{S}_1^*)$ and $(\mathbf{I}_n - \mathbf{S}_1^*\mathbf{S}_2^*)$ exist and thus the algorithm converges. \square

Proof of Corollary 1. It is easy to check that

$$\begin{aligned}
 &P(h > \max\{U_{[i+1]} - U_{[i]}, i = 1, \dots, n - 1\}, \bar{h} > \max\{V_{[i+1]} - V_{[i]}, i = 1, \dots, n - 1\}) \\
 &\geq 1 - P(h \leq \max\{U_{[i+1]} - U_{[i]}, i = 1, \dots, n - 1\}) \\
 &\quad - P(\bar{h} \leq \max\{V_{[i+1]} - V_{[i]}, i = 1, \dots, n - 1\}).
 \end{aligned} \tag{6}$$

Consider the second term above. We have

$$P(h \leq \max\{U_{[i+1]} - U_{[i]}, i = 1, \dots, n - 1\}) \leq \sum_{i=1}^{n-1} P(h \leq U_{[i+1]} - U_{[i]}). \tag{7}$$

Let F be the cumulative probability function of U . Then $U' = F(U)$ is uniformly distributed on $[0, 1]$. Let $U'_{[i]} = F(U_{[i]})$. By the joint distribution of $(U'_{[i]}, U'_{[i+1]})$ (see, e.g., David and Nagaraja (2003)) and simple calculation, we have, for any $c > 0$,

$$\begin{aligned}
 P(c \leq U'_{[i+1]} - U'_{[i]}) &= \int_{\tilde{u} > u+c} \frac{n!}{(i-1)!(n-i-1)!} u^{i-1} (1-\tilde{u})^{n-i-1} du d\tilde{u} \\
 &= \begin{cases} (1-c)^n, & \text{if } 0 \leq c \leq 1, \\ 0, & \text{if } c > 1. \end{cases}
 \end{aligned}$$

Let $c_0 = \inf\{f^{-1}(u), 0 \leq u \leq 1\}$, which is positive, by the assumption. Note that $U_{[i]} = G(U'_{[i]})$, where G is the inverse function of F . By the nature of inverse functions, we have $U_{[i+1]} - U_{[i]} \leq c_0(U'_{[i+1]} - U'_{[i]})$. Thus,

$$P(c_0 c \leq U_{[i+1]} - U_{[i]}) < P(c \leq U'_{[i+1]} - U'_{[i]}) = \begin{cases} (1-c)^{n-1}, & \text{if } 0 \leq c \leq 1, \\ 0, & \text{if } c > 1. \end{cases}$$

When n is large, we can assume $h < 1$. It follows that

$$\begin{aligned}
 \sum_{i=1}^{n-1} P(h \leq U_{[i+1]} - U_{[i]}) &\leq n(1-h)^{n-1} = n \exp\{(n-1) \log(1-h)\} \\
 &\leq n \exp\{(n-1)(-h + h^2/2)\} \leq n \exp\{-(n-1)h/2\} \\
 &\rightarrow 0
 \end{aligned} \tag{8}$$

as $n \rightarrow \infty$. The condition $nh / \log(n) \rightarrow \infty$ is used in the last step of (8). By (7) and (8), we have

$$P(h \leq \max\{U_{[i+1]} - U_{[i]}, i = 1, \dots, n - 1\}) \rightarrow 0$$

as $n \rightarrow \infty$. Similarly, we can show that

$$P(\bar{h} \leq \max\{V_{[i+1]} - V_{[i]}, i = 1, \dots, n - 1\}) \rightarrow 0$$

as $n \rightarrow \infty$. It follows from (6) and the two equations above that

$$P(h > \max\{U_{[i+1]} - U_{[i]}, i = 1, \dots, n-1\}, \hat{h} > \max\{V_{[i+1]} - V_{[i]}, i = 1, \dots, n-1\}) \rightarrow 1$$

as $n \rightarrow \infty$. By Remark 1 and (5), the algorithm converges in probability as $n \rightarrow \infty$. \square

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