PROBABILISTIC APPROACH TO THE SCHOENBERG SPLINE OPERATOR AND UNIMODAL DENSITY ESTIMATOR

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Abstract: Using Chebyshev's inequality, we provide a probabilistic proof of the uniform convergence for continuous functions on a closed interval by Schoenberg's variation diminishing spline operator. Furthermore, we introduce a unimodal density estimator based on this spline operator and thus generalize that of Bernstein polynomials and beta density. The advantage of this method is the local property. That is, refining the knots while keeping the degree fixed of B-splines yields better estimates. We also give a numerical example to verify our results.

1. Introduction

Although the Bernstein polynomials have been generalized in many different ways, see for example [5], [14], [13], the most striking one is the B–spline. Univariate spline functions are piecewise polynomials that are joined with certain continuity at their breakpoints. For nearly fifty years, spline functions have been so influential that not only they have played a central role in approximations but also provide an essential tool for mathematical sciences, such as computer aided geometric design and manufacturing see [8].

This work's contribution splits into two parts. First we amend the proofs of uniform convergence given by [15] which was based on the uniform knot sequence and that of [12] which relied on the Bohman-Korovkin's Theorem. In other words we provide a probabilistic view for the uniform convergence problem using the Schoenberg spline operator. A similar approach for the Bernstein polynomials was initiated in [2]. Secondly, we introduce a unimodal density estimator based on the Schoenberg spline operator to generalize both the Bernstein polynomials given by [16] and the beta density. We note that the classical approach for the problem of uniform convergence using spline functions employs the modulus of continuity to measure the maximum distance between the function and its approximation.

Schoenberg [15] introduced the following piecewise polynomial a variation diminishing operator as a generalization of the Bernstein operator,

$$S_k(f;x) = \sum_{j=-k}^{n-1} f(\overline{x}_{j,k}) N_{j,k}(x), \tag{1.1}$$

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with positive integers n, k and a non-decreasing (extended) knot sequence

$$T_{n,k} = (x_{-k} = \cdots = x_0 = 0 < x_1 < \cdots < x_n = \cdots = x_{n+k} = 1), \tag{1.2}$$

and $\overline{x}_{j,k} = (x_{j+1} + \cdots + x_{j+k})/k$. The set of functions

$$\{N_{j,k}(x) : 0 \le x \le 1, \quad j = -k, -k+1, \ldots, n-1\}$$

is the B-spline basis for the space of splines of degree k defined recursively by the de Boor algorithm, see [8],

$$N_{j,0}(x) = \begin{cases} 1, & \text{if } x \in [x_j, x_{j+1}) \\ 0, & \text{otherwise,} \end{cases}$$

$$N_{j,k}(x) = \frac{x - x_j}{x_{j+k} - x_j} N_{j,k-1}(x) + \frac{x_{j+k+1} - x}{x_{j+k+1} - x_{j+1}} N_{j+1,k-1}(x). \tag{1.3}$$

Note that the basis functions $N_{j,k}$ heavily depend on the knot sequence.

The operator $S_k f$ is positive, reproduces linear functions and is variation diminishing, and thus preserves and mimics the shape of f see for example [3, 9]. It is also proved in [12] that $S_k f$ converges to f uniformly for a continuous function on $[a, b]$ if and only if

$$\frac{\| T_{n,k} \|}{k} \to 0, \quad \text{where } \| T_{n,k} \| = \max_j (x_{j+1} - x_j).$$

The B-splines possess remarkable properties such as compact support, partition of unity, unimodality, refinability (breaking into simpler components) see [8, 1, 9, 11]. Bernstein–Bézier polynomials and B-splines have exerted a great influence over the development of geometric modelling and accelerated research in the analytical sciences.

The following identity attributed to Marsden, see [12], relates the monomial basis and the B-spline basis:

$$(t-x)^k = \sum_{j=-\infty}^{\infty} (t - x_{j+1}) \ldots (t - x_{j+k}) N_{j,k}(x), \tag{1.4}$$

where an empty product on the right denotes one.

2. Uniform convergence

We now proceed to the proof of uniform convergence of $S_k f$ to $f \in C[a, b]$ as $k \to \infty$. For clarity we take the interval $[0, 1]$. Consider $\xi_{n,k}$ as a sum of k independent random variables by $\xi_{n,k} = x_{j+1} + \cdots + x_{j+k}$ having probability mass function (PMF) $N_{j,k}(x)$ for $j = -k, \ldots, n-1$. Then the expectation E of $\xi_{n,k}$ is

$$E(\xi_{n,k}) = \sum_{j=-k}^{n-1} \xi_{n,k} N_{j,k}(x).$$

It follows from Marsden's identity by comparing the coefficients of t on both sides of (1.4) that $E(\xi_{n,k}) = kx$. Furthermore the variance of the random variable $\xi_{n,k}$ is

$$\text{Var}(\xi_{n,k}) = \sum_{j=-k}^{n-1} (\xi_{n,k} - kx)^2 N_{j,k}(x).$$

To find it, we write

$$\text{Var}(\xi_{n,k}) = k^2 \{ S_k(t^2; x) - 2x S_k(t; x) + x^2 S_k(1; x) \}.$$

We then obtain from (1.4) that

$$\mathrm{Var}(\xi_{n,k}) = \frac{1}{k-1} \sum_{j+1 \leq r < s \leq j+k} (x_s - x_r)^2 \leq \frac{k}{2} \max_{0 \leq j \leq n} (x_{j+k} - x_j)^2.$$

To estimate the distance between $S_k(f;x)$ and $f(x)$, let us examine

$$|S_k(f;x) - f(x)| \leq \sum_{j:|\frac{\xi_{n,k}}{k} - x| < \delta} |f(\frac{\xi_{n,k}}{k}) - f(x)| N_{j,k}(x)$$
$$+ \sum_{j:|\frac{\xi_{n,k}}{k} - x| \geq \delta} |f(\frac{\xi_{n,k}}{k}) - f(x)| N_{j,k}(x) := S_1 + S_2$$

From the uniform continuity of $f(x)$ on $[0,1]$ we can take δ so small that

$$|f(\frac{\xi_{n,k}}{k}) - f(x)| \leq \frac{\epsilon}{2} \text{ whenever } |\frac{\xi_{n,k}}{k} - x| < \delta.$$

Thus the first summation above satisfies $S_1 \leq \frac{\epsilon}{2}$. Since f is bounded on $[0,1]$, there is a positive constant M such that $|f(x)| \leq M$. Then

$$S_2 \leq 2M \sum_{j:|\frac{\xi_{n,k}}{k} - x| \geq \delta} N_{j,k}(x).$$

Notice that the sum on the right side of the last inequality is equal to the following probability with parameter x with respect to PMF of B-splines:

$$\sum_{j:|\frac{\xi_{n,k}}{k} - x| \geq \delta} N_{j,k}(x) = P_x(|\frac{\xi_{n,k}}{k} - x| \geq \delta).$$

By the Chebyshev inequality, see [6], the above probability satisfies

$$P_x(|\frac{\xi_{n,k}}{k} - x| \geq \delta) \leq \frac{\mathrm{Var}\left(\frac{\xi_{n,k}}{k}\right)}{\delta^2} = \frac{\mathrm{Var}(\xi_{n,k})}{k^2 \delta^2} \leq \frac{M}{k\delta^2} \leq \epsilon.$$

Finally choose $N \geq \frac{M}{\delta^2 \epsilon}$ such that $\frac{M}{k\delta^2} \leq \epsilon$.

We have thus proved the uniform convergence of sequences of Schoenberg operators:

THEOREM 1. *Given $\epsilon > 0$ and $f \in C[0,1]$, there exists an integer N such that*

$$\|S_k(f;x) - f(x)\| \leq \epsilon$$

for all $k \geq N$ and all $x \in [0,1]$.

Let us mention an important consequence of the theorem. First we recall the probabilistic interpretation of Jensen's inequality, see [6]. For a convex function f and a random variable X with a finite expectation $E(X)$, we have

$$f(E(X)) \leq E(f(X)).$$

Replacing $X = \overline{x}_{j,k}$ with probabilities $N_{j,k}(x)$ yields

$$f(E(X)) = f\left(\sum_{j=-k}^{n-1} \overline{x}_{j,k} N_{j,k}(x)\right) = f(x)$$

and

$$E(f(X)) = \sum_{j=-k}^{n-1} f(\overline{x}_{j,k}) N_{j,k}(x) = S_k(f;x).$$

Hence we obtain the following Corollary.

COROLLARY 1. *The approximation to a convex function $f(x)$ by $S_k(f;x)$ is one-sided, that is*

$$f(x) \leq S_k(f;x) \quad \text{for all } x \in [0,1] \quad \text{and for each } k \geq 1.$$

3. Unimodal estimator

The work [16] introduced a method of unimodal density estimation via Bernstein polynomials and beta density. We generalize their approach using the Schoenberg operator which replaces polynomials by B-splines. An important advantage of the latter is their local control property and refinement. In practice, for data or continuous approximation purposes while the degree of B-splines is fixed, we refine knot sequences at each stage until a desired outcome is attained. Cubic B-splines and uniform (equally spaced) knot sequences are common choices.

To establish a probability density function based on the B-splines, we require the following important fact about their integration (see for example [8]):

$$\int_{-\infty}^{+\infty} N_{j,k}(x)dx = \frac{1}{k+1}(x_{j+k+1} - x_j).$$

Now for each non-negative integer k, a positive integer n, and a given non-decreasing extended knot sequence similar to (1.2) and a function f on $[a,b]$, we define a new probability density function by

$$g_{n,k}(f,x) = \sum_{j=-k}^{n-1} \frac{k+1}{x_{j+k+1} - x_j} f(\overline{x}_{j,k}) N_{j,k}(x) \Big/ \left(\sum_{j=-k}^{n-1} f(\overline{x}_{j,k}) \right). \tag{3.1}$$

It is easy to verify that

$$\int_{-\infty}^{+\infty} g_{n,k}(f,x)dx = \int_a^b g_{n,k}(f,x)dx = 1.$$

This allows us to construct a family of unimodal density estimates

$$h_{n,k}(x,w) = \sum_{j=-k}^{n-1} w_j \frac{k+1}{x_{j+k+1} - x_j} N_{j,k}(x), \tag{3.2}$$

when weights satisfy the following properties:

1. $w_j \geq 0$ for each j and $\sum_{j=-k}^{n-1} w_j = 1$,

2. w is unimodal, i.e. there exists an integer m such that
$w_{-k} \leq w_{-k+1} \leq \cdots \leq w_m \geq w_{m+1} \geq \cdots \geq w_{n-1}$.
The equations (3.1) and (3.2) generalize the method given by [16] based on the Bernstein polynomials.

Special case: When $n = 1$, $N_{j,k}(x)$ with the knot sequence
$T_{n,k} = (0, \ldots, 0, 1, \ldots, 1)$ in which both 0 and 1 repeat $k+1$ times yields Bernstein basis polynomials of degree k on $[0,1]$,

$$\binom{k}{j} x^j (1-x)^{k-j}, \quad j = 0, 1, \ldots, k$$

or the Binomial distribution.

It follows that the density in (3.1) reduces to

$$g_{n,k}(f,x) = \sum_{j=0}^{k} (k+1)f(j/k)\binom{k}{j}x^j(1-x)^{k-j} \bigg/ \left(\sum_{j=0}^{k} f(j/k)\right),$$

the beta density function with shape parameters k and j. Therefore the functions on the right of (3.2), $(k+1)/(x_{j+k+1}-x_j)N_{j,k}(x)$ whose shape depend on j, k and a knot sequence T may be viewed as a generalization of the beta density.

Meanwhile we want to emphasize three references in a similar scope. The work [7] investigates urn models arising from the B-splines at non-negative integer knots and Karlins classic book on total positivity [10] has a blend of variation diminishing kernels, and the paper [4] focuses on optimality of B-splines.

4. Numerical examples

In this section, we present an example using simulated data to investigate the performance of proposed unimodal density estimation method. We explore this by generating data from Beta distribution with parameters 2 and 5 for the sample size 100. Then we choose weights w_j to construct the estimated density. The software R is used to carry out computations. The results compare the Bernstein polynomials estimation given by [16] and the proposed estimation with the beta density. In both methods, the Bernstein polynomials and B-splines keep the degree k fixed here we take $k=3$. Since the uniform knot sequence has been the most influential and widely implemented choice, $T_{n,k}$ is selected to be $(-0.6, -0.4, -0.2, 0, 0.2, 0.4, 0.6, 0.8, 1, 1.2, 1.4, 1.6)$.
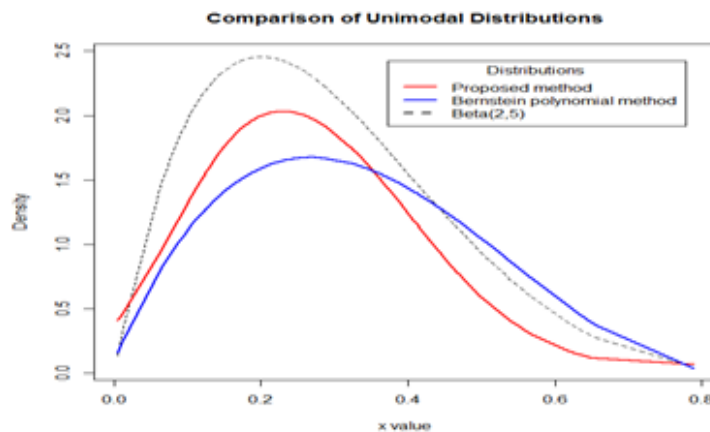

FIGURE 1. Comparison of unimodal distributions

In the Figure 1, we display the plot of Beta(2, 5), proposed estimator and Bernstein polynomials estimator of density function for the distribution. The graphs between true and estimated density functions show that the proposed estimator for the density function presents impressively smooth curve in the approximation of true distribution. MISE values of the proposed estimation function and Bernstein polynomials estimation function are obtained 0.1643 and 0.3554 respectively. MISE values of the proposed estimation function is reduced. It means that the proposed estimator is closer to the actual density function. The advantage of the proposed method is the local property, that is, refining the knots while keeping the degree fixed of B-splines yields better estimates. We also give another example to verify this property.

In this example, the number of knots is increased for the same data and the same degree and $T_{n,k}$ is taken as

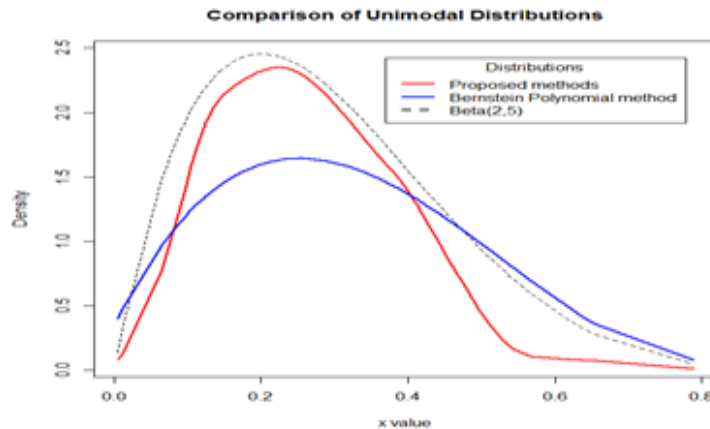$$(-0.15, -0.1, -0.05, 0, 0.05, 0.1, \ldots, 0, 9, 0.95, 1, 1.05, 1.1, 1.15).$$

FIGURE 2. Comparison of unimodal distributions refined knots

As shown in Figure 2, our unimodal density estimation method achieves a good approximation of true probability density function. The mean integrated squared error (MISE) of the proposed estimator value is 0.0701. When the number of knots increases, MISE of the proposed estimation function reduces. It means that the proposed estimator is closer to the actual density function. Thus, it is possible to make a better unimodal density estimate by taking increasing number of knots without changing the degree by means of our proposed method.

5. Conclusions

This work's contribution is in two parts. First we modify the proofs of uniform convergence which was based on the uniform knot sequence and that of [12] which relied on the Bohman-Korovkin's Theorem. In other words, we provide a probabilistic view of the uniform convergence problem using the Schoenberg spline operator. Secondly, we introduce a unimodal density estimator based on the B-splines to generalize both the Bernstein polynomials given by [16] and the beta density.

The above numerical examples demonstrate the effectiveness of our approach compared to the Bernstein polynomials method. Smaller of MISE values are obtained with our method. Furthermore, refining the knots of B-splines decreases MISE values while keeping the degree unchanged. This makes our method a suitable choice to achieve a better density estimation. A future area of interest is to extend this methodology to the cumulative distribution function.

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