Original Research Article

Rational splines with minimax parameters in nonparametric regression inverse problems

Abstract

It is considered a solution to curve-fitting problem by Spath rational spline. Here, parameters of spline are proposed to be calculated according to Chebyshev minimax principle. An algorithm of constructing such spline is proposed. An application to nonparametric regression is given that gives possibility to estimate unknown functions in stochastic differential equations. A case of SDE is given, with alpha-stable process. A software is developed and corresponding tests have been presented.

Keywords:Chebyshev approximation; splines; inverse problems; SDE

2010 Mathematics Subject Classification: 65K10; 65D05; 65D07; 65D15; 60H10

1 Introduction

A nonparametric estimation has become a powerful tool for the solution of different statistical and physical problems and can be efficiently used for estimating functions and functionals. Such models avoid restrictions on the form of estimated functions and give good results in cases where there are not many variables. In addition to classical problems such as density or regression function estimation, nonparametric methods can be used to estimate unknown functions in noise-independent statistical models.

One of the most important tools of nonparametric statistics is kernel estimation where a kernel function is introduced and used to construct a function estimator (Härdle (2004) , Tsybakov (2008) , Kvam, Vidakovic, and Kim (2022)). This approach has a drawback that sometimes it is difficult to calculate a bandwidth parameter to obtain a good estimator. Another approach is to use splines. Approximation splines are proposed in Reinsch (1967) and can be efficiently used to construct a good estimator. Another way is to use interpolation splines that can preserve the form of the curve.

In this article, an interpolation Spath rational spline is used (Späth (1995), Zavialov, Kvasov, and Miroshnichenko (1980)) that has two parameters on each subinterval. Here, parameters are proposed to be calculated according to the Chebyshev principle, which is the minimization of the maximum error between the given data and the fitted function. Chebyshev approximation has been studied in Dem'yanov and Malozemov (1990), Remez (1969), Popov and Tesler (1980) and, in most cases, the polynomial approximation is considered. In Popov (1989), rational splines are presented in a more general form. An algorithm for their construction is more complicated, and they are used only for approximation, without interpolation. An example of using splines in non-parametric regression is also considered, namely, for estimating unknown functions in stochastic differential equations.

The structure of the paper is as follows. The next section presents general information for rational spline and Chebyshev fitting. An algorithm for rational Spath spline construction with Chebyshevian parameters of tension is presented and numerical aspects are explained. The last section presents a developed software and the corresponding tests for models given by SDE.

2 Spline construction

Consider a curve-fitting problem when a grid $\Delta : a = x_0 < x_1 < ... < x_n = b$ is given on interval $[a, b]$ with correspondent function values $y_i, i = 0, ..., n$. The problem is to restore the function on the whole interval. One of the most well-known solutions to such a problem is spline fitting that besides a good approximation can preserve the form of the given function. When certain conditions are met, important properties, such as monotonicity and convexity, are preserved. One of the important classes of such splines is Spath rational spline (Späth (1995),Bogdanov and Volkov (2006)) that has the form on $[x_i, x_{i+1}]$:

$$S_R(x) = y_i(1-t) + y_{i+1}t + C_i\left(\frac{t^3}{1+p_i(1-t)} - t\right) + D_i\left(\frac{(1-t)^3}{1+q_it} - (1-t)\right),$$

where C_i, D_i coefficients, that are calculated by system of linear equations with threediagonal matrix, p_i, q_i are parameters that are called parameters of tension, $t = \dfrac{x - x_i}{h_i}$ and $h_i = x_{i+1} - x_i$

The advantage of a given spline is the availability of parameters $p_i, q_i \in (-1, \infty)$ that significantly affect the properties of the given spline. When $p_i, q_i \to 0$ the spline acquires properties of a cubic spline and when $p_i, q_i \to \infty$ the spline has properties of a linear spline. Several algorithms are proposed to calculate the parameters p_i, q_i. In Bogdanov and Volkov (2006) restrictions on parameters are proposed to preserve the monotonicity and convexity of the approximating function. In Frost and Kinzel (1982) the adjustment of the spline is completed by tensioning each internal section. In Schiess (1986) an algorithm for surfaces is proposed.

Here, the algorithm for constructing rational Spath spline is proposed, where tension parameters are calculated via the Chebyshev minimax principle.

The algorithm proposed in this article consists of two parts. Firstly, a rational Spath interpolation spline is constructed and then using Chebyshev approximation, parameters p_i, q_i are calculated.

In order to obtain an interpolation rational Spath spline, a system of linear equations with a three-diagonal matrix has to be solved. Following Zavialov et al. (1980), the tension parameters p_i, q_i have to be chosen in some way. Denote

$$\lambda_i = \frac{h_i}{(h_{i-1}+h_i)}, \mu_i = 1 - \lambda_i, P_{i-1} = \frac{3+3p_{i-1}+p_{i-1}^2}{(2+q_{i-1})(2+p_{i-1})-1}, Q_i = \frac{3+3q_i+q_i^2}{(2+q_i)(2+p_i)-1}$$

.

The system of equation wrt m_i that has to be solved has the form:

$$\lambda_iP_{i-1}m_{i-1} + (\lambda_iP_{i-1}(2+q_{i-1}) + \mu_iQ_i(2+p_i))m_i + \mu_iQ_im_{i+1} = \lambda_iP_{i-1}(3+q_{i-1})\frac{y_i - y_{i-1}}{h_{i-1}} + \mu_iQ_i(3+p_i)\frac{y_{i+1}-y_i}{h_i}, i = 1, 2, ...n-1 \quad (2.1)$$

This system is not full and has to be supplemented by two equations that are obtained from boundary conditions. The first type of these conditions will be used further, although the proposed algorithm does not depend on the boundary conditions :

$$Q_0(2+p_0)m_0 = Q_0(2+p_0)y_0', P_{n-1}(2+q_{n-1}m_n) = P_{n-1}(2+q_{n-1}y_n')$$

After obtaining values of m_i coefficients C_i, D_i are calculated by formulas:

$$C_i = \frac{-(3+q_i)(y_{i+1}-y_i) + h_i m_i + (2+q_i)h_i m_{i+1}}{(2+q_i)(2+p_i)-1}$$

$$D_i = \frac{(3+p_i)(y_{i+1}-y_i) - h_i m_{i+1} - (2+p_i)h_i m_i}{(2+q_i)(2+p_i)-1}$$

In this scheme, the parameters p_i, q_i are selected empirically, which does not always allow constructing a good approximation for a given function. In this article, it is proposed to select parameters according to the Chebyshev criterion, which minimizes the maximum deviation between the data and the approximating function. Suppose that interpolation is not carried out at all points, but in each interval h_i there are at least three pairs (x_i, y_i) of points that are not interpolated.

Chebyshev approximation is a solution to an optimization problem that has the form:

$$\min_a \max_{i=0,\ldots,n} |y_i - S(x_i;a)|$$

where $S(x;a)$ is a function approximation, a is the vector of unknown parameters that have to be estimated.

For solution to this problem a Remez algorithm can be used. Consider unknown function to be rational Spath spline with unknown parameters p_i, q_i. From $x = \{x_0, ..., x_n\}$ $m+1$ points $z = \{z_0, z_1, ..., z_m\}$ have to be chosen, where m is number of unknown parameters. These points have to form Chebyshev alternation that is:

$$r_m(z_0) = -r_m(z_1) = ... = (-1)^{m+1} r_m(z_{m+1})$$

where $r_m(z_j) = y_j - S(z_j; p_i, q_i)$. The following Remez algorithm with Valle-Poussin one-point change (Dem'yanov and Malozemov (1990)) can obtain an approximation that fits the Chebyshev criterion:

1. To choose initial values of z_i. This can be, for example, the roots of the Chebyshev polynomial. In the case of a discrete problem they can be calculated as:

$$z_i^0 = x_{r_i}, i = 0, 1, ..., m+1$$

where

$$r_i = \left[\frac{T-1}{2}\cos\frac{(m+1-i)\pi}{m} + \frac{T+1}{2}\right]$$

Here [.] is for the integer value.

2. To solve system of equations $y_i - F(z_i;a) = (-1)^i \mu$ and to determine vector of unknown parameters a and relative error μ

3. To check condition $\rho - |\mu| \leq \epsilon|\mu|$, where $\rho = max|r_m(x)|$, ϵ is precision. If it is satisfied, then end.

4. To change points of an alternation. In case of one-point change, one has to find out which x_i corresponds to ρ and enter it in alternation. Entering has to be without violation alternation condition, which means, that signums of $y_j - F(z_j;a)$ should be different. (see details in [7])

To sum up, an algorithm for constructing Spath spline with Chebyshev parameters of tension can be proposed:

1. For each interval $[x_i, x_{i+1}]$ choose start values p_i, q_i and to solve system of linear equations.

2. To calculate coefficients C_i, D_i.

3. Using Remez scheme to recalculate coefficients p_i, q_i on each interval $[x_i, x_{i+1}]$, where k is number of iteration.

4. To construct spline with recalculated coefficients p_i, q_i.

The main difficulty of this algorithm is that the system of equations that has to be solved in the second step is nonlinear. Instead of this this system can be turned into optimization problem of functional $F(z_i; p_i, q_i, \mu) = \sum_{i=1}^{3}(y_i - S(z_i; p_i, q_i) - (-1)^i)^2$. This problem can be solved, for example, by the Hooke-Jeeves algorithm [16], which is zero-order and does not require the calculation of derivatives.

3 Application to nonparametric regression

Given a discretely observed process that is a solution to the stochastic differential equation

$$\mathrm{d}X_t = A(X_t)\mathrm{d}t + \mathrm{d}Z_t, \tag{3.1}$$

where A - drift function, Z is symmetrical alpha-stable process with limited jumps. Observation is held with a constant step Δ.

Stochastic models generated by alpha-stable processes occur in financial modeling (Cont and Tankov (2003), Basegmez and Cekici (2017), Kyprianou (2006), Barbachan (2003), Wang, Li, Gao, and Meng (2015)), physics (Jha, Kaw, Kulkarni, Parikh, and Team (2003)), clymatology (Ditlevsen (1999)) etc. In Ditlevsen (1999) it was shown that the fast time scale noise forcing the climate contains a component with an alpha-stable distribution. Models, genereated by stochastic differential equations often contain unknown parameters that have to be estimated. In this article SDE driven by alpha-stable noise where drift function has unknown parameter is considered.

Consider process X that is a solution to the equation by Euler's method. Here, items of the model have the restriction that provides the existence and uniqueness of SDE's solution. Besides, it is assumed in simulations and obtaining numerical results there is a technical restriction that the jump value is bounded by some constant. Assume that the alpha-stable process with jumps Z has Lévy-Ito decomposition:

$$Z_t = ct + \int_0^t \int_{|u|>1} u\nu(\mathrm{d}s, \mathrm{d}u) + \int_0^t \int_{|u|\le 1} u\tilde{\nu}(\mathrm{d}s, \mathrm{d}u),$$

where ν – Poisson point measure with compensator $\mathrm{d}s\mu(\mathrm{d}u)$, $\tilde{\nu}(\mathrm{d}s, \mathrm{d}u) = \nu(\mathrm{d}s, \mathrm{d}u) - \mathrm{d}s\mu(\mathrm{d}u)$ is corresponding compensated measure. Following investigations in Bodnarchuk and Ivanenko (2016), Ivanenko and Kulik (2015), Ivanenko and Pogorielov (2023) it is assumed that ν satisfies the following conditions:

(i) For some $\kappa > 0$,

$$\int_{|u|\ge 1} u^{2+\kappa}\mu(du) < \infty;$$

(ii) For some $u_0 > 0$, the restriction μ on $[-u_0, u_0]$ has a positive density

$$\sigma \in C^2\left([-u_0, 0) \cup (0, u_0]\right);$$

(iii) There exists C_0 such that

$$|\sigma'(u)| \le C_0|u|^{-1}\sigma(u),$$
$$|\sigma''(u)| \le C_0 u^{-2}\sigma(u),$$
$$|u| \in (0, u_0];$$

(iv)

$$\left(\log\frac{1}{\epsilon}\right)^{-1}\mu\Big(\{u : |u| \ge \epsilon\}\Big) \to \infty, \quad \epsilon \to 0.$$

The proposed algorithm can be used to estimate unknown function A. Let X is a sample from the model given by SDE. Denote:

$$\bar{X}_j = \begin{cases} \dfrac{X_{j+1} - X_j}{h} & j = 1, 2...T-1 \\ \dfrac{X_j - X_{j-1}}{h} & j = T \end{cases}$$

Let $Y = \{y_0, ..., y_T\}$ to be unknown values of function in points of discretization, where T is number of observations. Than an estimator $\tilde{A}(\tilde{X}_j)$ for Y_j can be obtained solving the unconstrained optimization problem:

$$\tilde{A}(\tilde{X}_j) = \arg\min_{Y_j} \sum_{j=1}^{T-1} (\bar{X}_j - Y_j)^2$$

Following this it can be obtained estimators in other metrics:

$$L^1 : \tilde{A}(\tilde{X}_j) = \arg\min_{Y_j} \sum_{j=1}^{T-1} |\bar{X}_j - Y_j|$$

$$L^\infty : \tilde{A}(\tilde{X}_j) = \arg\min_{Y_j} \max_{j} |\bar{X}_j - Y_j|$$

For L^1 and L^2, a Hook-Jeeves method (Bazaraa, Sherali, and Shetty (2006)) can be used that is a zero-order method and does not require derivative calculation. In the case of the L^∞ problem obtained discreet min-max problem can be converted into the unconstrained problem:

$$\min_{Y \in \mathbb{R}^T} \nu^{-1} \log \sum_{j=1}^{T} \exp(\nu |\bar{X}_j - Y_j|)$$

where ν is the parameter that has a big value.

The solution to these optimization problems are drift estimators at points of discretization, and, therefore, regardless of the stochastic problem, it is necessary to restore the function by points on a certain interval. Here, a proposed algorithm can be used. As an example, two cases are considered. As a variance, a functional $\int_{min}^{max} (A(x) - \tilde{A}(x))^2 dx$ was chosen, where max, min are the highest and lowest values of X_i.

It has been developed software for nonparametric estimation of functions in stochastic differential equations. Here, a model that is given by SDE with alpha-stable noise is considered. A user can specify the number of observations, time step, start point, parameters for the alpha-stable process.The drift function is written by a symbolic line. An example of an interface is shown in the figure.

Example 1

Consider equation with drift function $A = -2x + \sin x$, number of observations $T = 400$, time step $\Delta = 1$, parameter $\alpha = 1.75$, starting point $X_0 = 1$. The unknown function is unbounded, with linear growth. It can be interpreted as a nontrivial case of the Ornstein-Uhlenbeck process because of the sinusoidal term in the drift function. The figure shows an example of an estimation. Here, A is the drift function and B is the estimator.

For 1000 experiments estimators have been constructed and the variance for L^2 estimator with rational minimax spline has been calculated. The figure shows the dependence of the variance on the number of observations. It can be concluded that the accuracy of approximation significantly depends on the number of observations, however, the complexity of calculation increases.

Figure 1: Estimation for drift function in first example

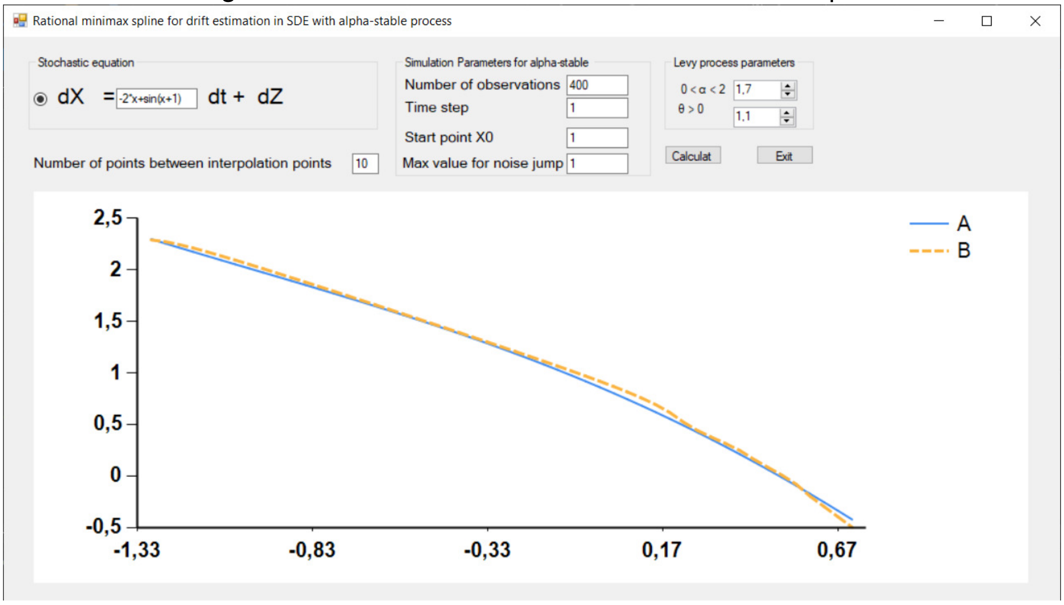
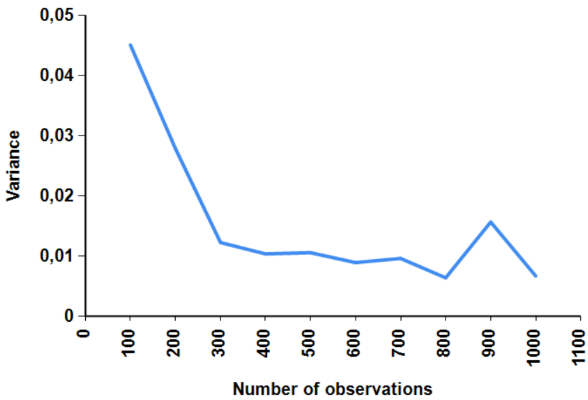


Figure 2: Variance dependence on number of observation in first example

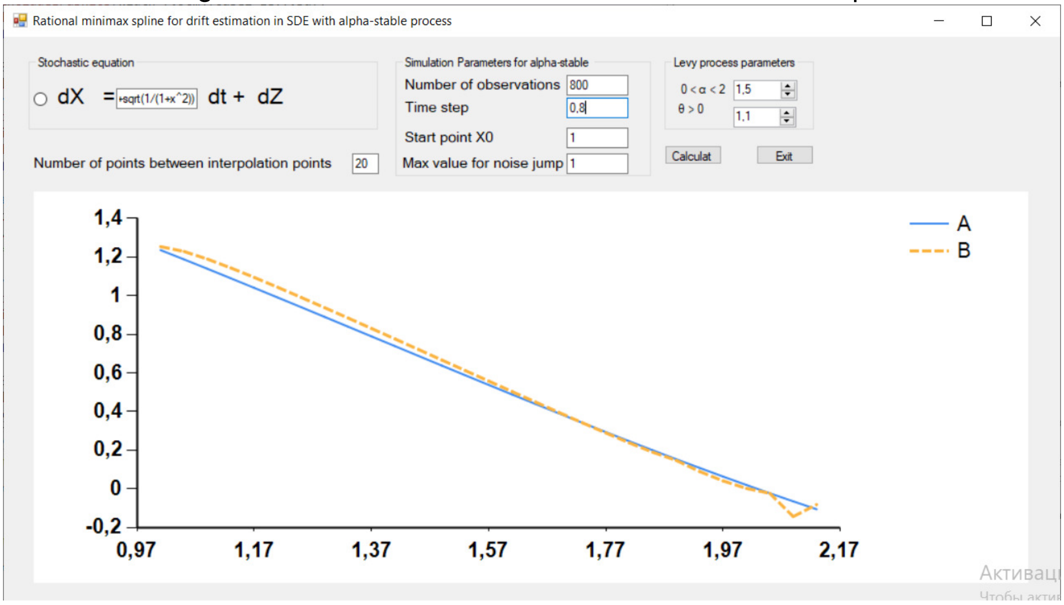


Example 2

Consider equation with drift function $A = \cos x + \sqrt{\dfrac{1}{1+x^2}}$, number of observations $T = 800$, time step $\Delta = 0.8$, parameter $\alpha = 1.5$, starting point $X_0 = 1$. In this example a bounded, periodical, nonlinear function is considered, with fluctuations.

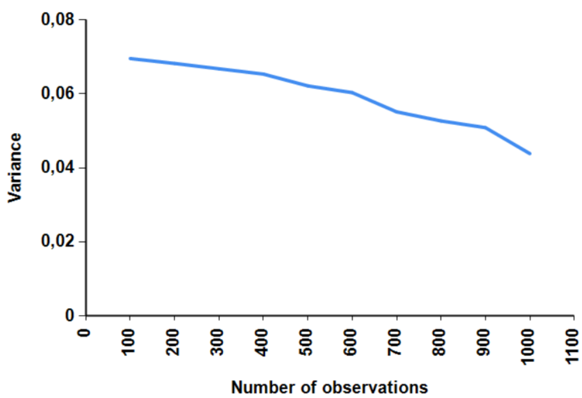
For 2000 experiments estimators have been constructed and the variance for L^1 estimator with

Figure 3: Estimation for drift function in second example



rational minimax spline has been calculated. The figure shows the dependence of the variance on the number of observations. It can be concluded that rational minimax spline is also suitable for nonlinear functions.

Figure 4: Variance dependence on number of observation in second example



It can be concluded that spline functions provide a good approximation for models with linear growth functions, as well as for periodic functions. Variance and bias decrease with the growth of the number of observations, which is a good property for an estimator.

4 Conclusions

As test results have shown, the Spath spline with minimax parameters can give a quite good approximation for different problems. Its main advantage is the absence of undersmoothing that appears in the case of spline interpolation. The variance decreases with an increasing number of observations, which is a property of a good estimator.

Different examples in models given by the solution of SDE show that the spline can approximate different classes of functions. In the first case, the drift function is an unbounded function with linear growth with nonlinearity. The second function is periodical, bounded, and nonlinear. As tests have shown, spline provides quite good an approximation and the variance and bias decrease with the growth of the number of observations.

5 Disclaimer (Artificial Intelligence)

Author hereby declare that NO generative AI technologies such as Large Language Models (ChatGPT, COPILOT, etc) and text-to-image generators have been used during writing or editing of manuscripts.

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