

A new SPH iterative method for solving nonlinear equations

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Abstract: In this paper, based on the basic principle of the SPH method's kernel approximation, a new kernel approximation was constructed to compute first order derivative through Taylor series expansion. Derivative in Newton's method was replaced to propose a new SPH iterative method for solving nonlinear equations. The advantage of this method is that it does not require any evaluation of derivatives, which overcame the shortcoming of Newton's method. Quadratically convergent of new method was proved and a variety of numerical examples were given to illustrate that the method has the same computational efficiency as the Newton's method.

Key words: SPH method; Nonlinear equations; Newton's method; Quadratically convergent; Iterative method.

1. Introduction

A variety of complex problems in different fields of science and engineering require finding the solution of a nonlinear equation (or the system of nonlinear equations) of the form $F(x) = 0$, in order to solve this equation researchers proposed many iterative methods [1–6]. Most of those methods were based on the well-known Newton's method, which is easy to implement and has quadratically convergence under fairly assumptions, however, it requires to compute $F'(x)$ with $F'(x) \neq 0$ in each calculation step, and some times it is difficult to provide the derivatives of function when the function is a complicated function. To overcome this problem, some derivative free iterative methods have been proposed [7–9].

In this paper, concerning derivative calculation in Newton's method, based on the basic principles of the smoothed particle hydrodynamics (SPH) [10, 11] method's kernel approximation, a new kernel approximation method was proposed to compute first order derivatives through Taylor series expansion. By replacing the derivatives in Newton's method, a new SPH iterative method was developed and the convergent of new method was proved. Several examples were calculated using the new method and the results were compared with Newton's method. Results showed that the new method almost has same accuracy and convergence with Newton's method.

2. Conventional SPH method

The first step of SPH method is the kernel approximation. The conventional kernel approximation for a function $f(x)$ and its derivatives at a particular point, whose position vector is x , in a volume Ω is defined as

$$\langle f(x) \rangle = \int_{\Omega} f(x') W(x - x', h) dx' \quad (1)$$

$$\langle \nabla f(x) \rangle = \int_{\Omega} f(x') \nabla W(x - x', h) dx' \quad (2)$$

Where $W(x - x', h)$ is kernel function and depends on two variable: distance of two points $|x - x'|$ and smoothing length h , which determines support domain of $W(x - x', h)$, the kernel function should satisfy some properties [12]. The most frequently used kernel function in SPH method is the cubic B-spline kernel. It has the form as shown in Eq.(3), Fig.1 shows that different smoothed length ($h = 1$ and $h = 0.5$ in one dimensional case) affects influence radius and shape of cubic B-spline kernel.

$$W(x - x', h) = \alpha_d \begin{cases} \frac{2}{3} - R^2 + \frac{1}{2}R^3 & 0 \leq R < 1 \\ \frac{1}{6}(2 - R)^3 & 1 \leq R < 2 \\ 0 & R \geq 2 \end{cases} \quad (3)$$

Where $\alpha_d = \frac{1}{h}, \frac{15}{7\pi h^2}, \frac{3}{2\pi h^3}$ in one, two and three dimensional cases respectively, R is the relative distance between two points (particles) at points x and x' , where $R = \frac{r}{h} = \frac{|x - x'|}{h}$ in which r is the distance between the two points.

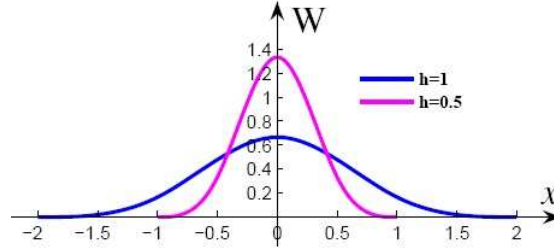


Fig. 1: **Figure of cubic B-spline kernel function in 1D case**

The second step of SPH method is the particle approximation, in which the problem domain is discretized into a finite number of randomly distributed particles which have mass and volume (see Fig. 2 For illustration in a two-dimensional case). Suppose infinitesimal volume dV' in the above integration at the location of j was replaced by the finite volume of the particle ΔV^j . If the particle mass and density are concerned, the ΔV^j can also be replaced by the corresponding mass to density ratio m^j/ρ^j ; the kernel approximation of a function and its derivatives expressed in Eq.(1) and Eq.(2) can be written in the following form of discretized particle approximation.

$$\langle f(x^i) \rangle = \sum_{j=1}^M \Delta V^j f^j W^{ij} = \sum_{j=1}^M \frac{m_j}{\rho_j} f^j W^{ij} \quad (4)$$

$$\langle \nabla f(x_i) \rangle = \sum_{j=1}^M \Delta V^j f^j \nabla W^{ij} = \sum_{j=1}^M \frac{m_j}{\rho_j} f^j \nabla W^{ij} \quad (5)$$

where $f^j = f(x^j)$, M is the number of particle in the support domain of particle i , $W^{ij} = W(x_i - x_j, h) = W(r^{ij}, h)$, $\nabla W^{ij} = \nabla W(x - x', h)|_{x=x^i, x'=x^j}$, $r^{ij} = |x^i - x^j|$

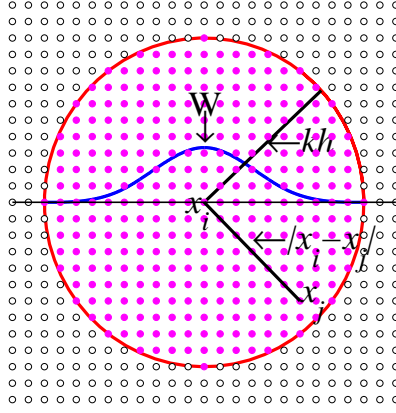


Fig. 2: SPH particle approximations

3. New kernel approximation method to compute first order derivatives

Let f be a function of variable x , f'' continuous and f''' exist in neighborhood of $x = x^i$, Taylor series expansion of f about the point $x = x^i$, retaining only three terms, written as

$$f(x) = f(x^i) + \frac{\partial f(x^i)}{\partial x_\alpha}(x_\alpha - x_\alpha^i) + \frac{1}{2} \frac{\partial^2 f(x^i)}{\partial x_\alpha \partial x_\beta}(x - x_\alpha^i)(x - x_\beta^i) + O[(x - x^i)^3] \quad (6)$$

where repeated indices α and β are summed over their ranges, but the repeated index i enclosed in parentheses is not summed.

By multiplying both sides of Eq.(6) with $(x_\gamma - x_\gamma^i)W(x - x^i, h)$ and integration of the resulting equation over the support domain Ω of kernel function $W(x - x^i, h)$ yields.

$$\begin{aligned} \int_{\Omega} f(x)(x_\gamma - x_\gamma^i)W(x - x^i, h)dx &= f(x^i) \int_{\Omega} (x_\gamma - x_\gamma^i)W(x - x^i, h)dx \\ &+ \frac{\partial f(x^i)}{\partial x_\alpha} \int_{\Omega} (x_\alpha - x_\alpha^i)(x_\gamma - x_\gamma^i)W(x - x^i, h)dx \\ &+ \frac{1}{2} \frac{\partial^2 f(x^i)}{\partial x_\alpha \partial x_\beta} \int_{\Omega} (x - x_\alpha^i)(x - x_\beta^i)(x_\gamma - x_\gamma^i)W(x - x^i, h)dx + O(h^4) \end{aligned} \quad (7)$$

Due to the symmetry of support domain Ω and the kernel function $W(x - x^i, h)$ is an even function, hence third integral on right hand side of Eq.(7) is equal to zero, therefore the Eq.(7) simplified to

$$\int_{\Omega} [f(x) - f(x^i)](x_\gamma - x_\gamma^i)W(x - x^i, h)dx = \frac{\partial f(x^i)}{\partial x_\alpha} \int_{\Omega} (x_\alpha - x_\alpha^i)(x_\gamma - x_\gamma^i)W(x - x^i, h)dx \quad (8)$$

By applying the particle approximation principle of SPH, from equation (8) leads to the following particle approximation of the derivative at a particle point i

$$\left\langle \frac{\partial f(x^i)}{\partial x_\alpha} \right\rangle = \left(\sum_{j=1}^M \frac{m^j}{\rho^j} x_\alpha^{ji} x_\gamma^{ji} W^{ji} \right)^{-1} \left(\sum_{j=1}^M \frac{m^j}{\rho^j} x_\gamma^{ji} f^{ji} W^{ji} \right) \quad (9)$$

where $x_\alpha^{ji} = x_\alpha^j - x_\alpha^i$, $x_\gamma^{ji} = x_\gamma^j - x_\gamma^i$, $f^{ji} = f(x^j) - f(x^i)$, $W^{ji} = W(x^j - x^i, h)$.

From the above Eq.(9) it can be seen that the calculation process of derivatives is not need to calculate the derivative of the kernel function. The kernel function could be used directly, reducing differentiability requirement of kernel function, at the same time a larger class of kernel functions could be used and the calculation is made easier.

3. The algorithm of new SPH iterative method

The famous Newton's methods is

$$x_{n+1} = x_n - [F'(x_n)]^{-1}F(x_n) \quad (10)$$

Applying new kernel approximation method introduced above into Eq.(10), get corresponding new SPH iterative method.

For numerical implementation of the presented method, provide the following algorithm.

Step 1: initial values of x_0 , tolerance ε , maximum number of iterations N , $n = 0$ and set the smooth length of kernel function h .

Step 2: while ($n \leq N$) do step(3-7)

Step 3: use Eq.(9) to compute $F'(x_n)$

Step 4: compute $y = -[F'(x_n)]^{-1}F(x_n)$

Step 5: $x_{n+1} = x_n + y$

Step 6: if $\|F(x_n)\| \leq \varepsilon$ or $\|x_{n+1} - x_n\| \leq \varepsilon$ output approximate solution x^* and stop

Step 7: set $n = n + 1$ and $x_n = x_{n+1}$

Step 8: output "the method failed after N iterations"; Stop

4. The convergent proof of new SPH iterative method

For the sake of simplicity only given and proved one variable case.

Theorem: Let $f''(x)$ continuous and $f'''(x)$ exist in neighborhood of $x = x^*$; and let $f(x^*) = 0$. The iterative method defined by equation (10) is quadratically convergent for smoothed length $h = K\Delta x$ and some Δx is sufficiently small.

Proof: In equation(9), if we use cubic B-spline kernel and set smoothed length $h = 1.1\Delta x$ in iterative process, the Eq.(10) will become following iterative formula accordingly

$$x_{n+1} = x_n - \frac{878\Delta x f(x_n)}{4[f(x_n + 2\Delta x) - f(x_n - 2\Delta x)] + 431[f(x_n + \Delta x) - f(x_n - \Delta x)]}$$

Let $e_n = x_n - x^*$, by using Taylor series expansion, we have

$$f(x_n) = e_n f' + \frac{1}{2} e_n^2 f'' + o(e_n^2)$$

$$f(x_n + \Delta x) = (e_n + \Delta x) f' + \frac{1}{2} (e_n + \Delta x)^2 f'' + o((e_n + \Delta x)^2)$$

$$f(x_n + 2\Delta x) = (e_n + 2\Delta x) f' + \frac{1}{2} (e_n + 2\Delta x)^2 f'' + o((e_n + 2\Delta x)^2)$$

here $f' = f'(x^*)$, $f'' = f''(x^*)$. Therefore, there holds

$$f(x_n + \Delta x) - f(x_n - \Delta x) = 2\Delta x[f' + e_n\Delta x f'' + o(e_n)]$$

so we have

$$\begin{aligned} e_{n+1} &= e_n - \frac{e_n f' + 1/2 e_n^2 f'' + o(e_n^2)}{f' + e_n \Delta x f'' + o(e_n)} \\ &= e_n^2 \frac{1/2 f'' + o(1)}{f' + e_n \Delta x f'' + o(e_n)} \end{aligned}$$

namely,

$$\lim_{n \rightarrow \infty} \frac{e_{n+1}}{e_n^2} = \frac{f''}{2f'}$$

which shows that the iterative method is at least a quadratically convergent.

5. Numerical examples

In this section presented some examples to illustrate the efficiency of the new SPH iterative method comparing with Newton's method (NM)(see Table1-3). In each example, the following stopping criteria was used.

$$\| F(x_n) \| \leq 10^{-15} \quad (11)$$

Computational order of convergence (COC) $\rightarrow \rho$ defined as:

$$\rho \approx \frac{\| x_{n+1} - x_n \| / \| x_n - x_{n-1} \|}{\| x_n - x_{n-1} \| / \| x_{n-1} - x_{n-2} \|} \quad (12)$$

Example 1: Application to one variable nonlinear equation

$$(1.1) x^2 - e^x - 3x + 2 = 0 \quad (1.2) \arctan x + \sin x + x - 2 = 0$$

$$(1.3) \sin^2 x - x^2 + 1 = 0 \quad (1.4) x^2 - (1 - x)^5 = 0$$

Example 2: Application to binary nonlinear equation

$$(2.1) \begin{cases} \frac{x}{\tan x} = -y \\ x^2 + y^2 = 3.5^2 \end{cases} \quad (2.2) \begin{cases} e^{x^2} + 8x \sin y = 0 \\ x + y = 1 \end{cases} \quad (2.3) \begin{cases} x^2 - 2x - y = -0.5 \\ x^2 + 4y^2 = 4 \end{cases}$$

Example 3: Application to ternary nonlinear equation

$$(3.1) \begin{cases} x^2 + y^2 + z^2 = 1 \\ 2x^2 + y^2 - 4z = 0 \\ 3x^2 - 4y^2 + z^2 = 0 \end{cases} \quad (3.2) \begin{cases} x^2 + y^2 + z^2 = 9 \\ xyz = 1 \\ x + y - z^2 = 0 \end{cases}$$

6. Conclusion

In this paper the SPH method used to finding roots of nonlinear equations and a new SPH iterative method for finding roots of nonlinear equations $F(x) = 0$ were proposed which has the following advantages:

- (1) This method is available for finding roots multiple dimensions equations.
- (2) The method only needs initial approximation of x_0 and it is not only need not to calculate any evaluation of derivatives of $F(x)$ and also need not to calculate of derivatives of kernel function $W(x - x', h)$.
- (3) The method is quadratically convergent and keep the same convergent and computational efficiency

Table 1: **Comparison of the presented method and Newton's methods to one variable nonlinear equation**

Examples	Root	Initial Value	Number of Iterations		COC— ρ	
			NM	SPH	NM	SPH
1.1	0.257530285439861	2	5	5	2.0006	2.0006
		-1	5	5	2.0007	2.0007
1.2	0.718586769063582	3	10	10	2.0007	2.0007
		0.1	5	5	1.9997	1.9997
1.3	1.404491648215340	2	5	5	2.0005	2.0005
		1	6	6	1.9999	1.9999
1.4	0.345954815848242	2	7	7	2.0012	2.0012
		-2	11	11	2.0004	2.0004

Table 2: **Comparison of the presented method and Newton's methods to binary nonlinear equation**

Examples	Root	Initial Value	Number of Iterations		COC— ρ	
			NM	SPH	NM	SPH
2.1	(2.389946943809752,	(3, 3)	8	8	1.9957	1.9957
	2.556981346387655)	(2, 2)	6	6	2.0003	2.0003
2.2	(-0.140285010811190,	(0.2, 0.8)	5	5	1.9997	1.9994
	1.140285010811190)	(-0.2, 2)	5	5	1.9621	1.9621
2.3	(-0.222214555059722,	(0.5, 0.5)	7	7	2.0015	2.0016
	0.993808418599834)	(0.5, 1.5)	5	5	1.9996	1.9996

Table 3: **Comparison of the presented method and Newton's methods to ternary nonlinear equation**

Examples	Root	Initial Value	Number of Iterations		COC— ρ	
			NM	SPH	NM	SPH
3.1	(0.560573416264006,	(0.5, 0.5, 0.5)	5	5	2.0000	2.0000
	0.497671169854288,	(1, 1, 1)	6	6	2.0065	2.0065
3.2	0.219040425836983)	(2.5, 0.5, 1.5)	5	5	1.9850	1.9850
	(2.491375696830689,	(2, 0.1, 2)	5	5	1.9183	1.9181
	0.242745878757136,					
	1.653517939300274)					

with the Newton method.

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