Numerical technique

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I. NUMEROV METHOD

The Taylor expansion of the function $f(x)$ up to 5th order is defined by

$$\begin{aligned} f(x) &= f(x_0) + (x-x_0)\left.\frac{\partial f(x)}{\partial x}\right|_{x=x_0} + \frac{1}{2}(x-x_0)^2\left.\frac{\partial^2 f(x)}{\partial x^2}\right|_{x=x_0} \\ &+\frac{1}{3!}(x-x_0)^3\left.\frac{\partial^3 f(x)}{\partial x^3}\right|_{x=x_0} + \frac{1}{4!}(x-x_0)^4\left.\frac{\partial^4 f(x)}{\partial x^4}\right|_{x=x_0} + \frac{1}{5!}(x-x_0)^5\left.\frac{\partial^5 f(x)}{\partial x^5}\right|_{x=x_0} + \mathcal{O}(h^6) \end{aligned} \tag{1}$$

If we define

$$f_n \equiv f(x_n) \tag{2}$$

$$f_{n+1} \equiv f(x_n + h) \tag{3}$$

$$f_{n-1} \equiv f(x_n - h) \tag{4}$$

then we obtain

$$f_{n+1} = f_n + h\left.\frac{\partial f(x)}{\partial x}\right|_n + \frac{1}{2}h^2\left.\frac{\partial^2 f(x)}{\partial x^2}\right|_n + \frac{1}{3!}h^3\left.\frac{\partial^3 f(x)}{\partial x^3}\right|_n + \frac{1}{4!}h^4\left.\frac{\partial^4 f(x)}{\partial x^4}\right|_n + \frac{1}{5!}h^5\left.\frac{\partial^5 f(x)}{\partial x^5}\right|_n + \mathcal{O}(h^6) \tag{5}$$

$$f_{n-1} = f_n - h\left.\frac{\partial f(x)}{\partial x}\right|_n + \frac{1}{2}h^2\left.\frac{\partial^2 f(x)}{\partial x^2}\right|_n - \frac{1}{3!}h^3\left.\frac{\partial^3 f(x)}{\partial x^3}\right|_n + \frac{1}{4!}h^4\left.\frac{\partial^4 f(x)}{\partial x^4}\right|_n - \frac{1}{5!}h^5\left.\frac{\partial^5 f(x)}{\partial x^5}\right|_n + \mathcal{O}(h^6) \tag{6}$$

The sum of (5) and (6) gives

$$f_{n+1} + f_{n-1} = 2f_n + h^2\left.\frac{\partial^2 f(x)}{\partial x^2}\right|_n + \frac{1}{12}h^4\left.\frac{\partial^4 f(x)}{\partial x^4}\right|_n + \mathcal{O}(h^6) \tag{7}$$

Now if we suppose $f(x)$ satisfies the differential equation,

$$\left[\frac{\partial^2}{\partial x^2} + V(x)\right] f(x) = 0 \tag{8}$$

Then (7) becomes

$$f_{n+1} + f_{n-1} = 2f_n - h^2 V(x_n) f_n + \frac{1}{12}h^4\left.\frac{\partial^4 f(x)}{\partial x^4}\right|_n + \mathcal{O}(h^6) \tag{9}$$

On the other hand, from (8), we can obtain

$$\begin{aligned} \frac{\partial^4 f(x)}{\partial x^4} &= -\frac{\partial^2}{\partial x^2}\left[V(x)f(x)\right] \\ &\sim -\frac{1}{h^2}\left[V(x_{n+1})f_{n+1} - 2V(x_n)f_n + V(x_{n-1})f_{n-1}\right] + \mathcal{O}(h^2) \end{aligned} \tag{10}$$

By inserting (10) into (9), we obtain

$$f_{n+1} + f_{n-1} = 2f_n - h^2 V(x_n) f_n - \frac{1}{12}h^2\left[V(x_{n+1})f_{n+1} - 2V(x_n)f_n + V(x_{n-1})f_{n-1}\right] + \mathcal{O}(h^6) \tag{11}$$

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Finally we obtain

$$\left(1+\frac{1}{12}h^2V(x_{n+1})\right)f_{n+1}-2\left(1-\frac{5}{12}h^2V(x_n)\right)f_n+\left(1+\frac{1}{12}h^2V(x_{n-1})\right)f_{n-1}=\mathcal{O}(h^6) \tag{12}$$

A. Numerical derivative

The difference of (5) and (6) gives

$$f_{n+1}-f_{n-1} \;=\; h\left.\frac{\partial f(x)}{\partial x}\right|_n+\frac{1}{3}h^3\left.\frac{\partial^3 f(x)}{\partial x^3}\right|_n+\mathcal{O}(h^5) \tag{13}$$

On the other hand, from (8), we can obtain

$$\begin{aligned}\left.\frac{\partial^3 f(x)}{\partial x^3}\right|_n &= -\left.\frac{\partial}{\partial x}\left[V(x)f(x)\right]\right|_n \\ &\sim -\frac{1}{2h}\left[V(x_{n+1})f_{n+1}-V(x_{n-1})f_{n-1}\right]+\mathcal{O}(h^2) \qquad \text{[3-point formula(27)]}\end{aligned} \tag{14}$$

By inserting (14) into (13), we obtain

$$\left.\frac{\partial f(x)}{\partial x}\right|_n = \frac{1}{h}\left[\left(1+\frac{1}{6}h^2V(x_{n+1})\right)f_{n+1}-\left(1+\frac{1}{6}h^2V(x_{n-1})\right)f_{n-1}\right]+\mathcal{O}(h^5) \tag{15}$$

Note that this is better approximation than the 5-point formula (36).

B. Bessel function

In the case of the spherical Bessel function ($f(x)\to F_l(x)=xj_l(x)$ or $xn_l(x)$), $V(x)$ of Eq.(8) is given by

$$V(x)=1-\frac{l(l+1)}{x^2}, \tag{16}$$

Eqs.(10) and (14), therefore, can be rewritten as

$$\begin{aligned}\frac{\partial^4 F_l(x)}{\partial x^4} &= -\frac{\partial^2}{\partial x^2}\left[V(x)F_l(x)\right]=-\left[\left(\frac{\partial^2 V(x)}{\partial x^2}-V^2(x)\right)F_l(x)+2\frac{\partial V(x)}{\partial x}\frac{\partial F_l(x)}{\partial x}\right] \\ &= \left\{\frac{6l(l+1)}{x^4}+\left(1-\frac{l(l+1)}{x^2}\right)^2\right\}F_l(x)-\frac{4l(l+1)}{x^3}\frac{\partial F_l(x)}{\partial x}\end{aligned} \tag{17}$$

$$\frac{\partial^3 F_l(x)}{\partial x^3} = -\frac{\partial}{\partial x}\left[V(x)F_l(x)\right]=-\left(\frac{\partial V(x)}{\partial x}F_l(x)+V(x)\frac{\partial F_l(x)}{\partial x}\right) \tag{18}$$

By inserting Eq.(17) into Eq.(9), one can obtain

$$\begin{aligned}F_l(x_{n+1})+F_l(x_{n-1}) &= \left[2-h^2\left(1-\frac{l(l+1)}{x_n^2}\right)+\frac{1}{12}h^4\left\{\frac{6l(l+1)}{x_n^4}+\left(1-\frac{l(l+1)}{x_n^2}\right)^2\right\}\right]F_l(x_n) \\ &\quad -\frac{1}{3}h^4\frac{l(l+1)}{x_n^3}\left.\frac{\partial F_l(x)}{\partial x}\right|_n+\mathcal{O}(h^6)\end{aligned} \tag{19}$$

II. THE LAGRANGE POLYNOMIAL METHOD

According to the Lagrange polynomial, the function $f(x)$ can be described by

$$f(x) \;\sim\; \sum_{k=0}^{n} f(x_k)L_k(x) \tag{20}$$

where

$$L_k(x) \;=\; \prod_{m(\neq k),0\leq m\leq n}\frac{x-x_m}{x_k-x_m} \tag{21}$$

By using this Lagrange polynomial, it is well known that n-point numerical derivative formula is given by

$$f'(x_j) \sim \sum_{k=0}^{n} f(x_k) L'_k(x_j) + \mathcal{O}(h^{n-1}) \tag{22}$$

where

$$L'_k(x_j) = \left.\frac{\partial L_k(x)}{\partial x}\right|_{x=x_j} \tag{23}$$

A. 3-points formula

We set 3-points as

$$f_n \equiv f(x_n) \tag{24}$$
$$f_{n+1} \equiv f(x_n + h) \tag{25}$$
$$f_{n-1} \equiv f(x_n - h) \tag{26}$$

Then we can obtain the numerical derivative formula by using (22),

$$f'(x_n) \sim f_{n-1} L'_{n-1}(x_n) + f_n L'_n(x_n) + f_{n+1} L'_{n+1}(x_n) + \mathcal{O}(h^2) = \frac{f_{n+1} - f_{n-1}}{2h} + \mathcal{O}(h^2) \tag{27}$$

where

$$L_{n-1}(x) = \frac{x - x_n}{x_{n-1} - x_n} \frac{x - x_{n+1}}{x_{n-1} - x_{n+1}} = \frac{1}{2h^2}(x - x_n)(x - x_{n+1}) \to L'_{n-1}(x_n) = -\frac{1}{2h} \tag{28}$$
$$L_n(x) = \frac{x - x_{n-1}}{x_n - x_{n-1}} \frac{x - x_{n+1}}{x_n - x_{n+1}} = -\frac{1}{h^2}(x - x_{n-1})(x - x_{n+1}) \to L'_n(x_n) = 0 \tag{29}$$
$$L_{n+1}(x) = \frac{x - x_{n-1}}{x_{n+1} - x_{n-1}} \frac{x - x_n}{x_{n+1} - x_n} = \frac{1}{2h^2}(x - x_{n-1})(x - x_n) \to L'_{n+1}(x_n) = \frac{1}{2h} \tag{30}$$

B. 5-points formula

We set 5-points as

$$f_n \equiv f(x_n) \tag{31}$$
$$f_{n+1} \equiv f(x_n + h) \tag{32}$$
$$f_{n-1} \equiv f(x_n - h) \tag{33}$$
$$f_{n+2} \equiv f(x_n + 2h) \tag{34}$$
$$f_{n-2} \equiv f(x_n - 2h) \tag{35}$$

Then we can obtain the numerical derivative formula by using (22),

$$\begin{aligned} f'(x_n) &\sim f_{n-2} L'_{n-2}(x_n) + f_{n-1} L'_{n-1}(x_n) + f_n L'_n(x_n) + f_{n+1} L'_{n+1}(x_n) + f_{n+2} L'_{n+2}(x_n) + \mathcal{O}(h^4) \\ &= \frac{1}{12h}\left(-f_{n+2} + 8f_{n+1} - 8f_{n-1} + f_{n-2}\right) + \mathcal{O}(h^4) \end{aligned} \tag{36}$$

where

$$L_{n-2}(x) = \frac{1}{24h^4}(x - x_{n-1})(x - x_n)(x - x_{n+1})(x - x_{n+2}) \to L'_{n-2}(x_n) = \frac{1}{12h} \tag{37}$$
$$L_{n-1}(x) = -\frac{1}{6h^4}(x - x_{n-2})(x - x_n)(x - x_{n+1})(x - x_{n+2}) \to L'_{n-1}(x_n) = -\frac{2}{3h} \tag{38}$$
$$L_n(x) = \frac{1}{4h^4}(x - x_{n-2})(x - x_{n-1})(x - x_{n+1})(x - x_{n+2}) \to L'_n(x_n) = 0 \tag{39}$$
$$L_{n+1}(x) = -\frac{1}{6h^4}(x - x_{n-2})(x - x_{n-1})(x - x_n)(x - x_{n+2}) \to L'_{n+1}(x_n) = \frac{2}{3h} \tag{40}$$
$$L_{n+2}(x) = \frac{1}{24h^4}(x - x_{n-2})(x - x_{n-1})(x - x_n)(x - x_{n+2}) \to L'_{n+2}(x_n) = -\frac{1}{12h} \tag{41}$$

III. STURMLIOUVILLE EQUATION AND NUMEROV METHOD.

The SturmLiouville equation takes the form,

$$\left[\frac{\partial}{\partial r}M(r)\frac{\partial}{\partial r}+U(r)\right]\phi(r)=\lambda\phi(r) \tag{42}$$

With this equation, if we suppose $u(r)$ which is the regular solution at the origin and $v(r)$ is the solution satisfies the out-going boundary condition respectively. The Wronskian W is defined by using $u(r)$ and $v(r)$,

$$W\equiv M(r)\left(u(r)\frac{\partial v(r)}{\partial r}-v(r)\frac{\partial u(r)}{\partial r}\right) \tag{43}$$

The derivative of the Wronskian is

$$\begin{aligned}\frac{\partial W}{\partial r} &= \frac{\partial}{\partial r}\left[M(r)\left(u(r)\frac{\partial v(r)}{\partial r}-v(r)\frac{\partial u(r)}{\partial r}\right)\right]\\ &= \frac{\partial M(r)}{\partial r}\left(u(r)\frac{\partial v(r)}{\partial r}-v(r)\frac{\partial u(r)}{\partial r}\right)+M(r)\left(u(r)\frac{\partial^2 v(r)}{\partial r^2}-v(r)\frac{\partial^2 u(r)}{\partial r^2}\right)\\ &= u(r)\frac{\partial M(r)}{\partial r}\frac{\partial v(r)}{\partial r}+u(r)M(r)\frac{\partial^2 v(r)}{\partial r^2}-v(r)\frac{\partial M(r)}{\partial r}\frac{\partial u(r)}{\partial r}-v(r)M(r)\frac{\partial^2 u(r)}{\partial r^2}\\ &= u(r)\frac{\partial}{\partial r}M(r)\frac{\partial}{\partial r}v(r)-v(r)\frac{\partial}{\partial r}M(r)\frac{\partial}{\partial r}u(r)=u(r)\left(\lambda-U(r)\right)v(r)-v(r)\left(\lambda-U(r)\right)u(r)=0\end{aligned} \tag{44}$$

Therefore $W=const$ for r.

If we take $\phi(r)\equiv M^{-\frac{1}{2}}(r)f(r)$,

$$\begin{aligned}\frac{\partial}{\partial r}M(r)\frac{\partial}{\partial r}\phi(r) &= \frac{\partial}{\partial r}M(r)\frac{\partial}{\partial r}M^{-\frac{1}{2}}(r)f(r)\\ &= M^{\frac{1}{2}}(r)\frac{\partial^2 f(r)}{\partial r^2}+\frac{1}{4}M^{-\frac{1}{2}}(r)\left[\frac{1}{M(r)}\left(\frac{\partial M(r)}{\partial r}\right)^2-2\frac{\partial^2 M(r)}{\partial r^2}\right]f(r)\end{aligned} \tag{45}$$

therefore (42) can be written by

$$\left[\frac{\partial^2}{\partial r^2}+\tilde{U}(r)\right]f(r)=\frac{\lambda}{M(r)}f(r) \tag{46}$$

where

$$\tilde{U}(r)=\frac{U(r)}{M(r)}+\frac{1}{4M(r)}\left[\frac{1}{M(r)}\left(\frac{\partial M(r)}{\partial r}\right)^2-2\frac{\partial^2 M(r)}{\partial r^2}\right] \tag{47}$$

By replacing $u(r)=M^{-\frac{1}{2}}(r)f(r)$ and $v(r)=M^{-\frac{1}{2}}(r)g(r)$, the Wronskian becomes

$$\begin{aligned}W &\equiv M(r)\left(u(r)\frac{\partial v(r)}{\partial r}-v(r)\frac{\partial u(r)}{\partial r}\right)\\ &= M(r)\left(u(r)\frac{\partial}{\partial r}M^{-\frac{1}{2}}(r)g(r)-v(r)\frac{\partial}{\partial r}M^{-\frac{1}{2}}(r)f(r)\right)\\ &= M(r)\left(M^{-\frac{1}{2}}(r)f(r)\frac{\partial}{\partial r}M^{-\frac{1}{2}}(r)g(r)-M^{-\frac{1}{2}}(r)g(r)\frac{\partial}{\partial r}M^{-\frac{1}{2}}(r)f(r)\right)\\ &= \left(f(r)\frac{\partial}{\partial r}g(r)-g(r)\frac{\partial}{\partial r}f(r)\right)\end{aligned} \tag{48}$$