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B-splines and Bernstein basis polynomial

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Description of B-splines

B-splines $B_i^{(k)}(r)$, $i = 1, 2, \ldots, N$ are piecewise polynomial functions of order k, completely defined by a set of points $\{t_j\}$, $j = 1, 2, \ldots, N + k$ which may be in part coincident

$$r_{min} = t_1 \leq \cdots \leq t_{N+k} = r_{max}$$

The common choice is to make the end-points of the support grid k-fold degenerate

$$\begin{aligned} t_1 &= \cdots = t_k \quad = r_{min} \\ t_{N+1} &= \cdots = t_{N+k} = r_{max} \end{aligned}$$

The knot sequence defines the extent of individual splines.
B-splines of the order $k > 1$ are defined recursively by the Cox - de Boor relation

$$B_i^{(k)}(r) = \frac{r - t_i}{t_{i+k-1} - t_i} B_i^{(k-1)}(r) + \frac{t_{i+k} - r}{t_{i+k} - t_{i+1}} B_{i+1}^{(k-1)}(r)$$

supplemented with the definition of B-splines of the order $k = 1$

$$B_i^{(1)}(r) = \begin{cases} 1, & \text{for } \; t_i \leq r < t_{i+1} \\ 0, & \text{for } \; r < t_i, \; r \geq t_{i+1} \end{cases}$$

The recursion is numerically stable and allows to define and manipulate B-splines of arbitrary order and knot point distribution

- Each spline $B_i^{(k)}(r)$ expands over an interval $[t_i, t_{i+k})$, which contains k subintervals, and is indexed by the knot i, $i = 1, \cdots, N$, where it starts

- Splines $B_i^{(k)}(r)$ are polynomials of the maximum degree $n = k - 1$

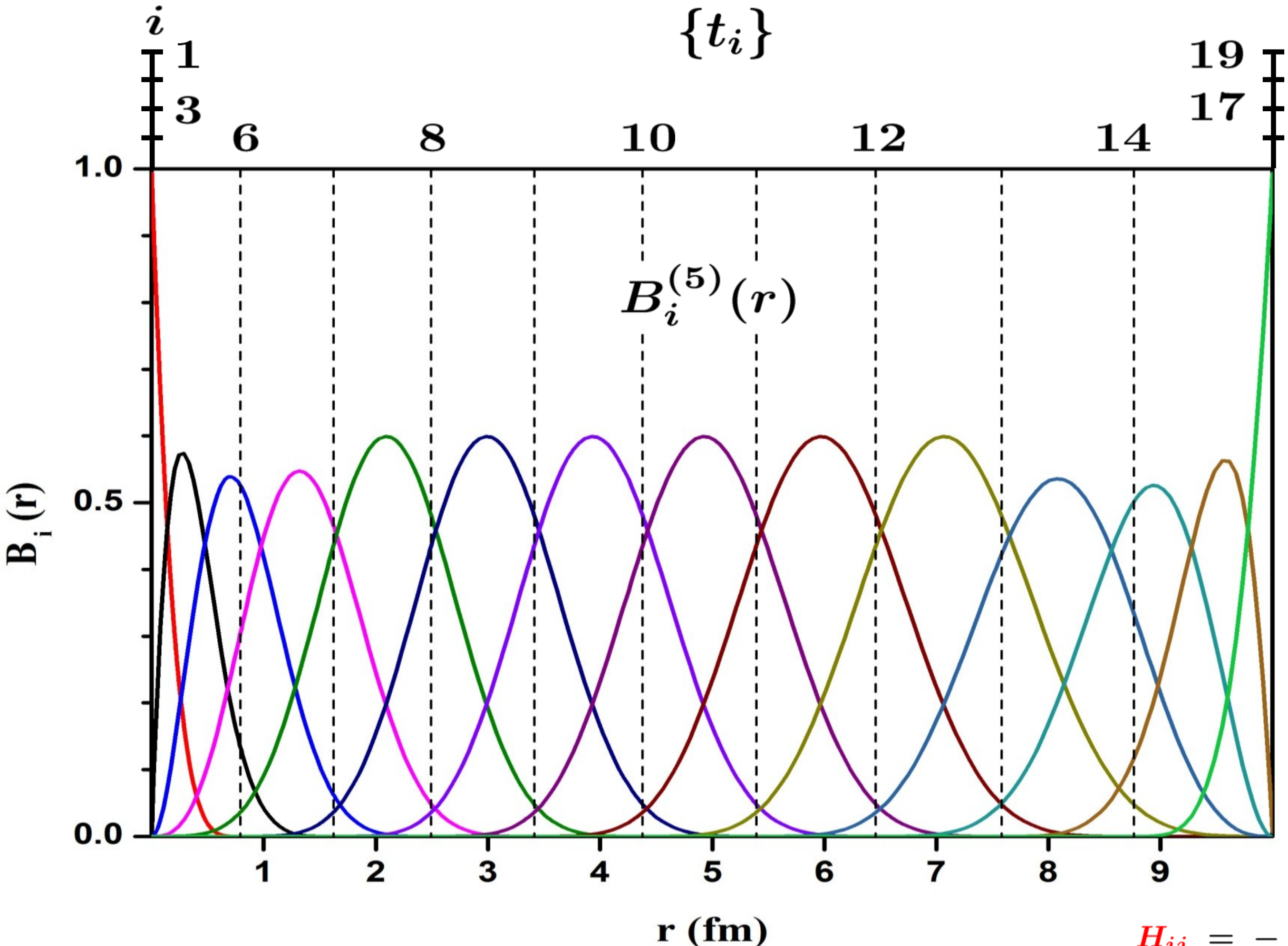
- The sum of B-splines represents the partition of the unity
  $\sum_{i=1}^{N} B_i^{(k)}(r) = 1$ for the radial interval $r_{min} \le r \le r_{max}$
  The set of B-splines of the order k and the knot sequence $\{t_j\}$ forms
  a complete basis for piecewise polynomials of the degree n
  on the radial interval spanned by the knot sequence

- The derivative of a B-spline of the order k can be expressed as a linear combination of B-splines of the order $(k - 1)$

- All B-splines are non-negative functions with convex shapes

- An arbitrary function $f(r)$ in this interval can be decomposed over B-splines

$$f(r) = \sum_{i=1}^{N} c_i \, B_i^{(k)}(r) = \sum_{j=i-k+1}^{i} c_j \, B_j^{(k)}(r), \text{ for } r \in [t_i, t_{i+1}]$$



$$\psi(r) = \sum_i c_i \, B_i^{(k)}(r)$$

$$\sum_j H_{ij} \, c_j = E \sum_j S_{ij} \, c_j$$

$$\begin{pmatrix}
\star & \star & \star & & & & & & & & & \\
\star & \star & \star & \star & & & & & & & & \\
\star & \star & \star & \star & \star & & & & & & & \\
 & \star & \star & \star & \star & \star & & & & 0 & & \\
 & & \star & \star & \star & \star & \star & & & & & \\
 & & & \star & \star & \star & \star & \star & & & & \\
 & & & & \star & \star & \star & \star & \star & & & \\
 & & & & & \star & \star & \star & \star & \star & & \\
 & & & & & & \star & \star & \star & \star & \star & \\
 & & 0 & & & & & \star & \star & \star & \star & \star \\
 & & & & & & & & \star & \star & \star & \star \\
 & & & & & & & & & \star & \star & \star
\end{pmatrix}$$

$$\begin{aligned}
H_{ij} &= -\int_0^{r_{max}} B_i^{(k)}(r)\, \frac{d^2}{dr^2}\, B_j^{(k)}(r) dr \\
&+ \int_0^{r_{max}} B_i^{(k)}(r)\, \frac{l(l+1)}{r^2}\, B_j^{(k)}(r) dr \\
&+ \int_0^{r_{max}} B_i^{(k)}(r)\, 2V(r)\, B_j^{(k)}(r) dr \\
S_{ij} &= \int_0^{r_{max}} B_i^{(k)}(r)\, B_j^{(k)}(r) dr
\end{aligned}$$

- de Boor C. A Practical Guide to Splines.
  New York: Springer, 1978
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  The use of basis splines in theoretical atomic physics
  J. Phys B: 1996. V. 29. P. 5213
- Bachau H. et al.,
  Applications of B-splines in atomic and molecular physics
  Rep. Prog. Phys. 2001. V. 64. P. 1815

Derivation of the B-spline analytical representation

To get the analytical presentation $\Rightarrow$ scale a radial dependence to a variable x_i which is a common for all subintervals $[t_i, t_{i+1})$

$$x_i = \frac{r - t_i}{t_{i+1} - t_i}, \quad \text{for} \quad t_i \le r < t_{i+1}$$

$$1 - x_i = \frac{t_{i+1} - r}{t_{i+1} - t_i}, \quad \text{where} \quad 0 \le x_i < 1$$

Subinterval i can be selected by a projector operator $\delta_i \equiv B_i^{(1)}(r) = 1$ for $t_i \le r < t_{i+1}$

$$\delta_i * \delta_j = \begin{cases} \delta_i, & i = j \\ 0, & i \ne j \end{cases}$$

A set of constant $z_{l,\,m}^{i,\,j}$ which depends on the grid $\{t_j\}$ can be defined

$$z_{l,\,m}^{i,\,j} = \frac{t_i - t_j}{t_l - t_m}, \quad l \ne m \qquad z_{l,m}^{i,i} = 0 \; ; \; z_{l,m}^{l,m} = 1$$

Factors before B-splines in the Cox - de Boor recurrence relation

$$\frac{r - t_i}{t_{i+n} - t_i} = \sum_{j=0}^{n-1} \delta_{i+j} \quad \left(z_{i+n,\,i}^{i+j,\,i} + z_{i+n,\,i}^{i+j+1,\,i+j} \, x_{i+j} \right)$$

$$\frac{t_{i+n+1} - r}{t_{i+n+1} - t_{i+1}} = \sum_{j=0}^{n-1} \delta_{i+j+1} \left(z_{i+n+1,\,i+1}^{i+n+1,\,i+j+2} + z_{i+n+1,\,i+1}^{i+j+2,\,i+j+1} \, (1 - x_{i+j+1}) \right)$$

It follows from the Cox - de Boor recurrence relation

B-spline on any subinterval $i \Rightarrow \begin{cases} \text{a sum of products from two factors,} \\ x_i \text{ and } (1 - x_i), \text{ taken in different powers} \end{cases}$

The Bernstein basis function $b_l^{(m)}(x)$ for $l = 0, 1, \cdots, m$ is the m-th degree polynomial

$$b_l^{(m)}(x) = \binom{m}{l} x^l (1-x)^{m-l}, \quad 0 \le x \le 1, \quad \binom{m}{l} = \frac{m!}{l!\,(m-l)!}$$

$$b_1^{(1)}(x) = x \ , \ b_0^{(1)}(x) = 1 - x$$

These functions form a complete basis over interval $[0, 1]$

Thus, B-splines of the order $(n+1)$ can be presented by an analytic form via Bernstein basis functions of the n-th degree

$$B_i^{(n+1)}(r) = \sum_{j=0}^{n} \delta_{i+j} \sum_{l=0}^{n} c_{j,l}^{i,n}\, b_l^{(n)}(x_{i+j})$$

The aim is to find unknown coefficients $c_{j,l}^{i,n}$ that depend only on a distribution of the grid points $\{t_j\}$ and a degree of B-spline polynomials n

Coefficients $c_{j,l}^{i,n}$ are obtained by recurrence relations for three regions $[t_i, t_{i+1}]$, $[t_{i+1}, t_{i+2}, \cdots, t_{i+n}]$ and $[t_{i+n}, t_{i+n+1}]$ where a spline $B_i^{(n+1)}(r)$ is non-zero

$\underline{j = 0,\ \text{region}\ [t_i, t_{i+1}]}$

$$
\begin{aligned}
c_{0,l}^{i,n} &= 0, \quad \text{for} \quad l = 0, 1, \cdots, (n-1) \\
c_{0,n}^{i,n} &= z_{i+n,i}^{i+1,i} * c_{0,n-1}^{i,n-1} = z_{i+n,i}^{i+1,i} * z_{i+n-1,i}^{i+1,i} * \cdots * z_{i+1,i}^{i+1,i}
\end{aligned}
$$

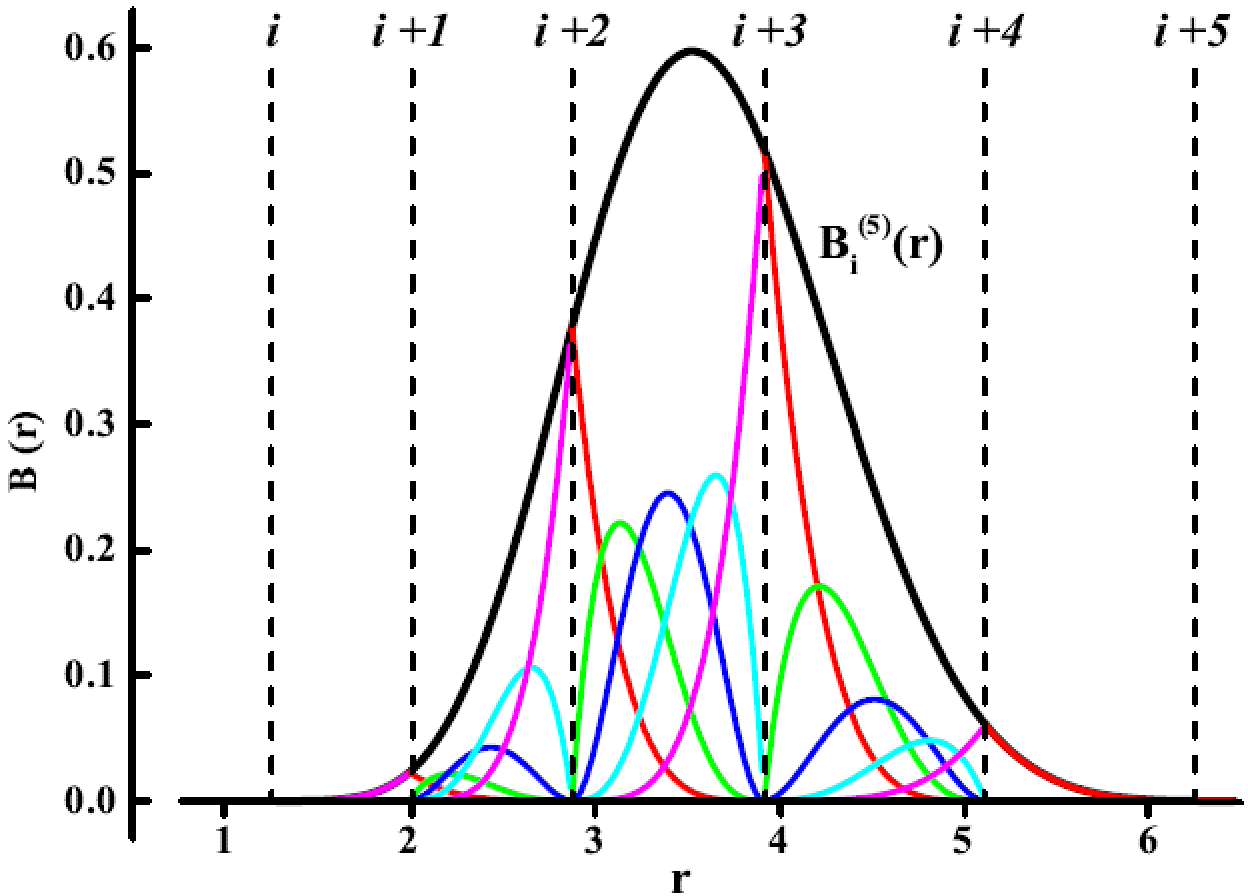
$\underline{j = \mathrm{n},\ \text{region}\ [t_{i+n}, t_{i+n+1}]}$

$$
\begin{aligned}
c_{n,0}^{i,n} &= z_{i+n+1,i+1}^{i+n+1,i+n} * c_{n-1,0}^{i,n-1} = z_{i+n+1,i+1}^{i+n+1,i+n} * z_{i+n+1,i+2}^{i+n+1,i+n} * \cdots * z_{i+n+1,i+n}^{i+n+1,i+n} \\
c_{n,l}^{i,n} &= 0, \quad \text{for} \quad l = 1, \cdots, n
\end{aligned}
$$

$\underline{j = 1, 2, \cdots, n-1,\ \text{regions}\ [t_{i+1}, t_{i+2}, \cdots, t_{i+n}]}$

$$
\begin{aligned}
c_{j,l}^{i,n} &= \left(\frac{n-l}{n}\right)\left(z_{i+n,i}^{i+j,i} * c_{j,l}^{i,n-1} + z_{i+n+1,i+1}^{i+n+1,i+j} * c_{j-1,l}^{i+1,n-1}\right) \\
&+ \left(\frac{l}{n}\right)\left(z_{i+n,i}^{i+j+1,i} * c_{j,l-1}^{i,n-1} + z_{i+n+1,i+1}^{i+n+1,i+j+1} * c_{j-1,l-1}^{i+1,n-1}\right)
\end{aligned}
$$

$$
B_i^{(k)}(r) = \frac{r - t_i}{t_{i+k-1} - t_i} B_i^{(k-1)}(r) + \frac{t_{i+k} - r}{t_{i+k} - t_{i+1}} B_{i+1}^{(k-1)}(r)
$$



i
i +1
i +2
i +3
i +4
i +5
0.6
0.5
0.4
0.3
0.2
0.1
0.0
B (r)
$B_i^{(5)}(r)$
1
2
3
4
5
6
r

Bernstein basis functions and Bernstein polynomials

- Lorentz G. G. Bernstein Polynomials. Toronto: University of Toronto Press, 1953.
- Phillips G. M. Interpolation and Approximation by Polynomials. New York: Springer, 2003.

Bernstein basis functions $b_l^{(m)}(x) = \binom{m}{l} x^l \, (1-x)^{m-l}, \quad 0 \leq x \leq 1$

- The Bernstein basis functions are positive $b_l^{(m)}(x) \geq 0$
- satisfy symmetry relation $b_l^{(m)}(x) = b_{m-l}^{(m)}(1-x)$
- partition of the unity $\sum_{l=0}^{m} b_l^{(m)}(x) = 1$ on interval $[0,1]$ for any degree m
- Bernstein function $b_l^{(m)}(x)$ has a unique local maximum at point $x = l/m$
- An arbitrary Bernstein basis polynomial can be written in terms of Bernstein polynomials of higher degree

$$b_l^{(m-1)}(x) = \frac{m-l}{m}\, b_l^{(m)}(x) + \frac{l+1}{m}\, b_{l+1}^{(m)}(x)$$

- $b_l^{(m-1)}(x)$ can be calculated by the numerically stable recurrence relation

$$\begin{aligned} b_l^{(m)}(x) &= x\, b_{l-1}^{(m-1)}(x) + (1-x)\, b_l^{(m-1)}(x) \\ b_1^{(1)}(x) &= x, \quad b_0^{(1)}(x) = 1 - x \end{aligned}$$

- The first and second derivatives of the m-th degree Bernstein basis function

$$\frac{db_l^{(m)}(x)}{dx} = m\left(b_{l-1}^{(m-1)}(x) - b_l^{(m-1)}(x)\right)$$

$$\frac{d^2b_l^{(m)}(x)}{dx^2} = m(m-1)\left(b_{l-2}^{(m-2)}(x) - 2b_{l-1}^{(m-2)}(x) + b_l^{(m-2)}(x)\right)$$

- multiplication of two Bernstein functions gives again the Bernstein basis function

$$b_l^{(m)}(x) * b_j^{(k)}(x) = \frac{\binom{m}{l}\binom{k}{j}}{\binom{m+k}{l+j}}\, b_{l+j}^{(m+k)}(x)$$

- An indefinite integral of Bernstein basis is given by a sum of the Bernstein basis functions of degree $(m+1)$

$$\int b_l^{(m)}(x)\,dx = \frac{1}{m+1}\sum_{j=l+1}^{m+1} b_j^{(m+1)}(x)$$

- all Bernstein basis functions of the same order have the same definite integral over interval $[0,1]$

$$\int_0^1 b_l^{(m)}(x)\,dx = \frac{1}{m+1}, \quad \text{for } l = 0, 1, \cdots, m$$

Function $f(x)$ (continuous on the interval $[0,1]$) can be approximated by the Bernstein polynomials $\mathcal{B}_m(f;x)$

$$f(x) \simeq \mathcal{B}_m(f;x) = \sum_{l=0}^{m} f_{m,l}\, b_l^{(m)}(x) \; ; \; f_{m,l} = f\,(l/m)$$

$f_{m,l}$ is a value of the function $f(x)$ at the point $x = (l/m)$ where basis polynomial $b_l^{(m)}(x)$ has the maximum

The sequence of Bernstein polynomials $\mathcal{B}_m(f;x)$ converges uniformly to the function $f(x)$ on interval $[0,1]$ with increasing of the order m. Convergence can be increased significantly by iterated Bernstein polynomials

$$f(x) \simeq \mathcal{B}_m^{(k)}(f;x) = \sum_{l=0}^{m} f_{m,l}^{(k)}\, b_l^{(m)}(x)$$

$$f_{m,l}^{(k+1)} = \sum_{i=0}^{m} f_{m,i}^{(k)} \left(\delta_{i,l} - b_i^{(m)}(l/m)\right) + f_{m,l} \; , \; k > 1$$

$$f_{m,l}^{(2)} = \sum_{i=0}^{m} f_{m,i} \left(2\,\delta_{i,l} - \; b_i^{(m)}(l/m)\right)$$

$$f_{m,l}^{(3)} = \sum_{i=0}^{m} f_{m,i} \left(3\,\delta_{i,l} - 3\,b_i^{(m)}(l/m) + \sum_{j=0}^{m} b_i^{(m)}(j/m)\, b_j^{(m)}(l/m)\right)$$

The 'optimal' Bernstein polynomial approximation corresponds to the limit $k \to \infty$

$$f_{m,l}^{(\infty)} = \sum_{i=0}^{m} f_{m,i} \left(b_i^{(m)}(l/m)\right)^{-1}_{i,l}$$

Guan Z. Iterated Bernstein polynomial approximations, arXiv 0909.0684

Sum Rules

From an unity partition by B-splines follows sum rule for coefficients $c_{j,l}^{i,n}$

$$\frac{1}{n+1} \sum_{i=j-n}^{j} \sum_{l=0}^{n} c_{j-i,l}^{i,n} = 1$$

average value of a B-spline $B_i^{(n+1)}(r)$ over its support interval is independent of i and thus is independent of the choice of the knots

$$\frac{1}{(t_{i+n+1}-t_i)} \int_{t_i}^{t_{i+n+1}} dr\, B_i^{(n+1)}(r) = \frac{1}{n+1} \Rightarrow \sum_{j=0}^{n} z_{i+n+1,\,i}^{i+j+1,\,i+j} \sum_{l=0}^{n} c_{j,l}^{i,n} = 1$$

Overlap integrals

overlap integral between two B-splines, $B_{i_1}^{(n+1)}(r)$ and $B_{i_2}^{(n+1)}(r)$ with $|i_1 - i_2| \le n$

$$\langle B_{i_1}^{(n+1)} | B_{i_2}^{(n+1)} \rangle = \int_{r_{min}}^{r_{max}} dr\, B_{i_1}^{(n+1)}(r)\, B_{i_2}^{(n+1)}(r)$$

$$\langle B_{i_1}^{(n+1)} | B_{i_2}^{(n+1)} \rangle = \sum_{j_1=0}^{n-i_1+i_2} \frac{(t_{i_1+j_1+1} - t_{i_1+j_1})}{(2n+1)} \sum_{l_1,l_2=0}^{n} c_{j_1,l_1}^{i_1,n} * c_{i_1-i_2+j_1,l_2}^{i_2,n} \binom{n}{l_1}\binom{n}{l_2}\binom{2n}{l_1+l_2}^{-1}$$

The similar expressions can be derived for other overlap integrals $\langle B_{i_1}^{(n+1)'} | B_{i_2}^{(n+1)'} \rangle$ and $\langle B_{i_1}^{(n+1)} | B_{i_2}^{(n+1)''} \rangle$

Matrix elements

the function $f(r)$ can be approximately written on grid $[r_{min}, r_{max}]$ as

$$f(r) \simeq \sum_j \delta_j \, \mathcal{B}_{N_j}(f; x_j) = \sum_j \delta_j \sum_{l=0}^{N_j} f_{N_j,l} \, b_l^{(N_j)}(x_j)$$

$$f_{N_j,l} = f\left(t_j + (t_{j+1} - t_j)\frac{l}{N_j}\right), \quad x_j = \frac{r - t_j}{t_{j+1} - t_j}$$

Matrix elements of the function $f(r)$ between two B-splines ($B_{i_1}^{(n+1)}(r)$ and $B_{i_2}^{(n+1)}(r)$) set up the banded symmetric matrix, which has non-zero elements for indices $|i_1 - i_2| \leq n$, corresponding to B-splines with the common support domain

$$\langle B_{i_1}^{(n+1)} | f | B_{i_2}^{(n+1)} \rangle = \int_{r_{min}}^{r_{max}} dr \, B_{i_1}^{(n+1)}(r) \, f(r) \, B_{i_2}^{(n+1)}(r)$$

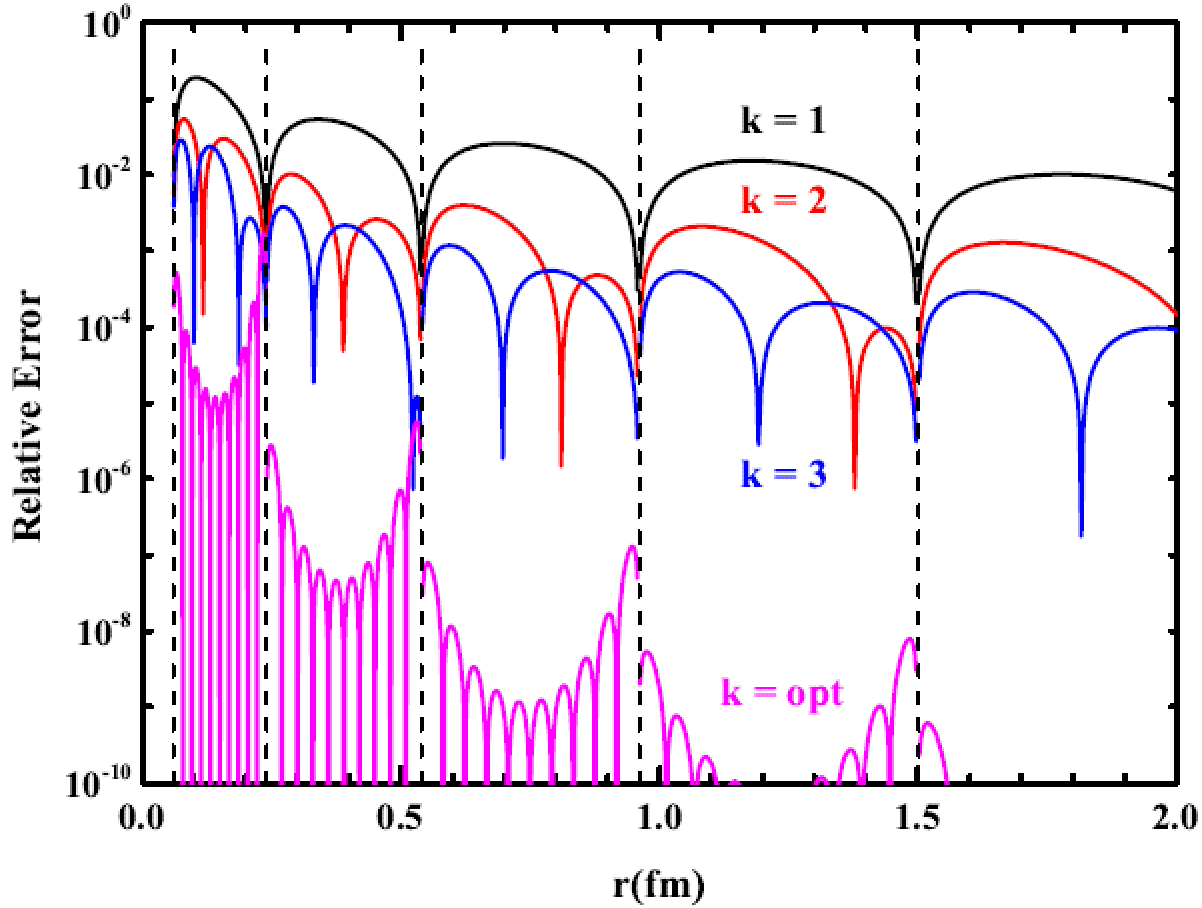
$$= \sum_{j_1=0}^{n-i_1+i_2} (t_{i_1+j_1+1} - t_{i_1+j_1}) \sum_{l_1,l_2=0}^{n} c_{j_1,l_1}^{i_1,n} * c_{i_1-i_2+j_1,l_2}^{i_2,n} \binom{n}{l_1}\binom{n}{l_2} F_{l_1+l_2}^{i_1+j_1}$$

Coefficients F_l^j, $l = 0, 1, \cdots, 2n$ equal to

$$F_l^j = \frac{1}{(2n + N_j + 1)} \sum_{m=0}^{N_j} f_{N_j,m} \binom{N_j}{m}\binom{2n + N_j}{l + m}^{-1}$$

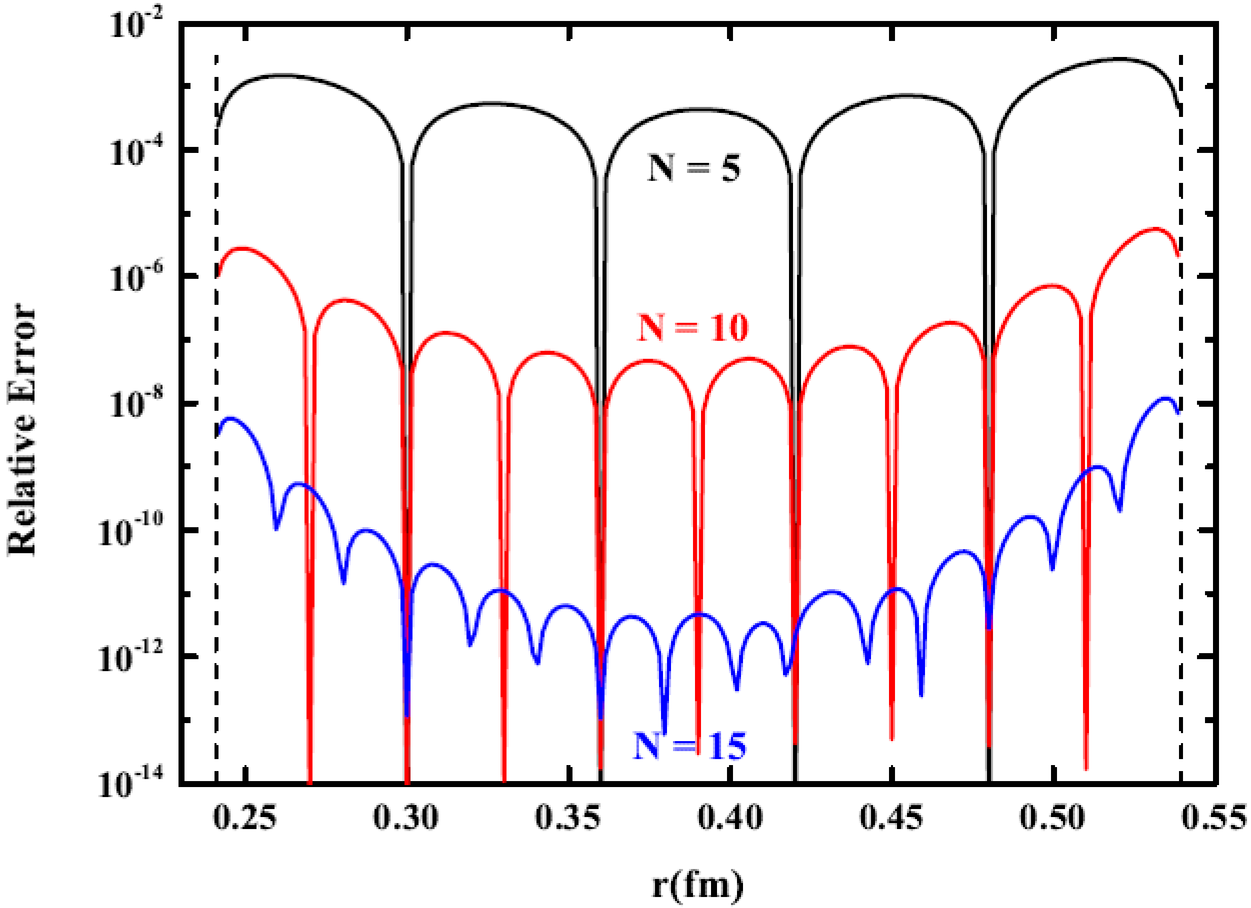
This method of calculations is rather flexible.
The integration over a radial variable is performed exactly.
Total accuracy depends on the precision of function approximation,
which can be additionally accelerated by using the iterated Bernstein polynomials

approximation of the function $f(r) = \dfrac{1}{r^2}$ by the iterated Bernstein polynomials with $N_j = 10$ for the first, second, third iterations and the optimal approximation



$$\text{Relative Error} = \left| \left(f(r) - \mathcal{B}_{N_j}^{(k)}(f; x_j) \right) / f(r) \right|$$

The optimal function approximation for $f(r) = \dfrac{1}{r^2}$ by the iterated Bernstein polynomials with $N_j = 5$, 10 and 15. The vertical dashed lines are boundaries of the interval $[t_j, t_{j+1}]$



$$\text{Relative Error} = \left| \left(f(r) - \mathcal{B}_{N_j}^{(k)}(f; x_j) \right) / f(r) \right|$$

Summary and conclusion

- B-splines are one of the most commonly used family of piecewise polynomials, which are well adapted to numerical tasks
- The analytic representation for B-splines of the arbitrary degree $(n+1)$ and arbitrary sets of the knot sequence via a decomposition on Bernstein basis polynomials $b_l^{(n)}(x)$ of the n-th degree was derived
- After the knot sequence of B-splines is constructed, the decomposition coefficients $c_{j,\,l}^{i,\,n}$ must be calculated only once
- Bernstein basis polynomials have remarkable analytic properties that allows to perform analytically many mathematical operations with B-splines
- If necessary, the iterated Bernstein polynomials can be used to accelerate the convergence
- This expands an applicability and enhances a flexibility of B-spline methods