

Theorems for Polynomial Interpolation

Fundamental Theorem of Algebra

Every non-zero, single-variable, degree n polynomial has, counted with multiplicity, at most n roots.

Existence and Uniqueness of Polynomial Interpolation

Given $(x_i, y_i)_{i=0}^n$, with x_i 's distinct. There exists one and only polynomial $P_n(x)$ of degree $\leq n$ such that $P_n(x_i) = y_i$ for all $i = 0, 1, \dots, n$.

Proof: Existence: by construction.

Uniqueness: Assume we have two polynomials $p(x), q(x) \in \mathcal{P}_n$, such that

$$p(x_i) = y_i, \quad q(x_i) = y_i, \quad i = 0, 1, \dots, n$$

Now, let $g(x) = p(x) - q(x)$, a polynomial of degree $\leq n$.

$$g(x_i) = p(x_i) - q(x_i) = y_i - y_i = 0, \quad i = 0, 1, \dots, n$$

So $g(x)$ has $n + 1$ zeros. By the Fundamental Theorem of Algebra, we must have $g(x) \equiv 0$, therefore $p(x) \equiv q(x)$.

Error Theorem for Polynomial Interpolation

Given a function $f(x)$ on $x \in [a, b]$, and a set of distinct points $x_i \in [a, b]$, $i = 0, 1, \dots, n$. Let $P_n(x) \in \mathcal{P}_n$ s.t.,

$$P_n(x_i) = f(x_i), \quad i = 0, 1, \dots, n$$

error function : $e(x) = f(x) - P_n(x), \quad x \in [a, b]$.

Theorem. There exists some value $\xi \in [a, b]$, such that

$$e(x) = \frac{1}{(n+1)!} f^{(n+1)}(\xi) \prod_{i=0}^n (x - x_i), \quad \text{for all } x \in [a, b]$$

Proof. If $f \in \mathcal{P}_n$, then by Uniqueness Theorem of polynomial interpolation we must have $f(x) = P_n(x)$. Then $e(x) \equiv 0$ and the proof is trivial.

Now assume $f \notin \mathcal{P}_n$. If $x = x_i$ for some i , we have $e(x_i) = f(x_i) - P_n(x_i) = 0$, and the result holds.

Now consider $x \neq x_i$ for any i .

$$W(x) = \prod_{i=0}^n (x - x_i) \in \mathcal{P}_{n+1},$$

it holds

$$W(x_i) = 0, \quad W(x) = x^{n+1} + \dots, \quad W^{(n+1)} = (n+1)!$$

Fix an y such that $a \leq y \leq b$ and $y \neq x_i$ for any i . We define a constant

$$c = \frac{f(y) - P_n(y)}{W(y)}$$

and another function

$$\varphi(x) = f(x) - P_n(x) - cW(x).$$

We find all the zeros for $\varphi(x)$. We see that x_i 's are zeros since

$$\varphi(x_i) = f(x_i) - P_n(x_i) - cW(x_i) = 0, \quad i = 0, 1, \dots, n$$

and also y is a zero because

$$\varphi(y) = f(y) - P_n(y) - cW(y) = 0$$

Here goes our deduction:

$\varphi(x)$ has at least	$n + 2$	zeros on $[a, b]$.
$\varphi'(x)$ has at least	$n + 1$	zeros on $[a, b]$.
$\varphi''(x)$ has at least	n	zeros on $[a, b]$.
	\vdots	
$\varphi^{(n+1)}(x)$ has at least	1	zero on $[a, b]$. Call it ξ s.t. $\varphi^{(n+1)}(\xi) = 0$.

So we have

$$\varphi^{(n+1)}(\xi) = f^{(n+1)}(\xi) - 0 - cW^{(n+1)}(\xi) = 0.$$

Recall $W^{(n+1)} = (n+1)!$, we have, for every y ,

$$f^{(n+1)}(\xi) = cW^{(n+1)}(\xi) = \frac{f(y) - P_n(y)}{W(y)}(n+1)!.$$

Writing y into x , we get

$$e(x) = f(x) - P_n(x) = \frac{1}{(n+1)!} f^{(n+1)}(\xi) W(x) = \frac{1}{(n+1)!} f^{(n+1)}(\xi) \prod_{i=0}^n (x - x_i),$$

for some $\xi \in [a, b]$.

Example of Error Formula

Recall the error formula: $e(x) = \frac{1}{(n+1)!} f^{(n+1)}(\xi) \prod_{i=0}^n (x - x_i)$

Example 1. If $n = 1$, $x_0 = a$, $x_1 = b$, $b > a$, find an upper bound for error.

Answer. Let

$$M = \max_{a \leq x \leq b} |f''(x)| = \|f''\|_{\infty}$$

and observe

$$\max_{a \leq x \leq b} |(x-a)(x-b)| = \dots = \frac{(b-a)^2}{4}.$$

For $x \in [a, b]$, we have

$$|e(x)| = \frac{1}{2} |f''(\xi)| \cdot |(x-a)(x-b)| \leq \frac{1}{2} \|f''\|_{\infty} \frac{(b-a)^2}{4} = \frac{1}{8} \|f''\|_{\infty} (b-a)^2.$$

Error depends on the distribution of nodes x_i .

Uniform Grid.

Equally distribute the nodes (x_i) : on $[a, b]$, with $n+1$ nodes.

$$x_i = a + ih, \quad h = \frac{b-a}{n}, \quad i = 0, 1, \dots, n.$$

One can show that for $x \in [a, b]$, it holds

$$\prod_{i=0}^n |x - x_i| \leq \frac{1}{4} h^{n+1} \cdot n!$$

Proof. If $x = x_i$ for some i , then $x - x_i = 0$ and the product is 0, so it trivially holds. Now assume $x_i < x < x_{i+1}$ for some i . We have

$$\max_{x_i < x < x_{i+1}} |(x - x_i)(x - x_{i+1})| = \frac{1}{4} (x_{i+1} - x_i)^2 = \frac{h^2}{4}.$$

Now consider the other terms in the product, say $x - x_j$, for either $j > i+1$ or $j < i$. Then

$|x - x_j| \leq h(j-i)$ for $j > i+1$ and $|x - x_j| \leq h(i+1-j)$ for $j < i$. In all cases, the product of these terms are bounded by $h^{n-1}n!$, proving the result.

We have the error estimate

$$|e(x)| \leq \frac{1}{4(n+1)} |f^{(n+1)}(x)| h^{n+1} \leq \frac{M_{n+1}}{4(n+1)} h^{n+1}$$

where

$$M_{n+1} = \max_{x \in [a, b]} |f^{(n+1)}(x)| = \|f^{(n+1)}\|_{\infty}$$

Chebyshev nodes: equally distributing the error

Type I: including the end points. For interval $[-1, 1]$: $\bar{x}_i = \cos\left(\frac{i}{n}\pi\right)$, $i = 0, 1, \dots, n$ For

interval $[a, b]$: $\bar{x}_i = \frac{1}{2}(a+b) + \frac{1}{2}(b-a)\cos\left(\frac{i}{n}\pi\right)$, $i = 0, 1, \dots, n$. One can show that

$$\max_{a \leq x \leq b} \left\{ \prod_{k=0}^n |x - \bar{x}_k| \right\} = 2^{-n} \leq \max_{a \leq x \leq b} \left\{ \prod_{k=0}^n |x - x_k| \right\}$$

where x_k is any other choice of nodes.

Error bound: $|e(x)| \leq \frac{1}{(n+1)!} \|f^{(n+1)}(x)\|_{\infty} 2^{-n}$.

Splines (Optional)

Intro

General Idea: Using piecewise polynomials to approximate the function.

Given a set of data

x	t_0	t_1	\cdots	t_n
y	y_0	y_1	\cdots	y_n

Find a function $\mathcal{S}(x)$ which interpolates the points $(t_i, y_i)_{i=0}^n$. The set $t_0 < t_1 < \cdots < t_n$ are called knots. Note that they need to be ordered. $\mathcal{S}(x)$ consists of piecewise polynomials

$$\mathcal{S}(x) \doteq \begin{cases} \mathcal{S}_0(x), & t_0 \leq x \leq t_1 \\ \mathcal{S}_1(x), & t_1 \leq x \leq t_2 \\ \vdots \\ \mathcal{S}_{n-1}(x), & t_{n-1} \leq x \leq t_n \end{cases}$$

$\mathcal{S}(x)$ is called a spline of degree k , if

- $\mathcal{S}_i(x)$ is a polynomial of degree k ;
- $\mathcal{S}(x)$ is $(k-1)$ times continuous differentiable, i.e., for $i = 1, 2, \dots, k-1$ we have

$$\begin{aligned} \mathcal{S}_{i-1}(t_i) &= \mathcal{S}_i(t_i), \\ \mathcal{S}'_{i-1}(t_i) &= \mathcal{S}'_i(t_i), \\ &\vdots \\ \mathcal{S}_{i-1}^{(k-1)}(t_i) &= \mathcal{S}_i^{(k-1)}(t_i), \end{aligned}$$

Commonly used splines:

- $n = 1$: linear spline (simplest)
- $n = 2$: quadratic spline (less popular)
- $n = 3$: cubic spline (most used)

Numerical Integration

Problem Description: Given a function $f(x)$, defined on an interval $[a, b]$, we want to find an approximation to the integral

$$I(f) = \int_a^b f(x) dx.$$

Main ideas:

- Cut up $[a, b]$ into smaller sub-intervals;
- In each sub-interval, find a polynomial $p_i(x) \approx f(x)$;
- Integrate $p_i(x)$ on each sub-interval, and sum them up.

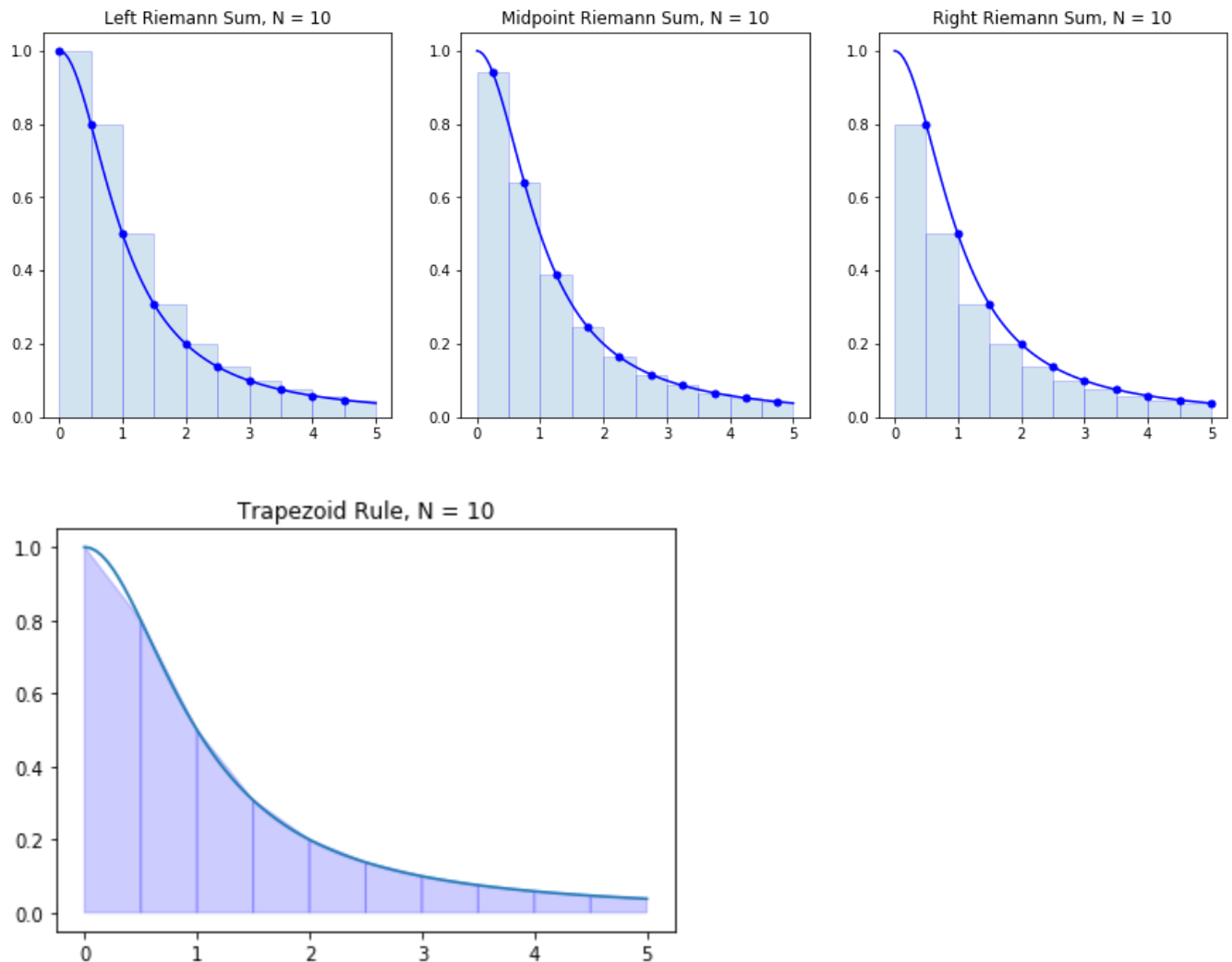


Image Source: Mathematical Python

Trapezoid Rule on Uniform Grid: $\int_a^b f(x)dx \approx h \left[\frac{1}{2} f(x_0) + \sum_{i=1}^{n-1} f(x_i) + \frac{1}{2} f(x_n) \right]$

Error estimate for trapezoid rule

Intermediate Value Theorem : In mathematical analysis, the intermediate value theorem states that if f is a continuous function whose domain contains the interval $[a, b]$, then it takes on any given value between $f(a)$ and $f(b)$ at some point within the interval.

We define the error:

$$E(f; h) \doteq I(f) - T(f; h) = \sum_{i=0}^{n-1} \int_{x_i}^{x_{i+1}} [f(x) - p_i(x)] dx = \sum_{i=0}^{n-1} E_i(f; h),$$

where $E_i(f; h)$ is the error on each sub-interval

$$E_i(f; h) = \int_{x_i}^{x_{i+1}} [f(x) - p_i(x)] dx, \quad (i = 0, 1, \dots, n-1)$$

Error bound with polynomial interpolation:

$$f(x) - p_i(x) = \frac{1}{2} f''(\xi_i) (x - x_i) (x - x_{i+1}), \quad (x_i < \xi_i < x_{i+1})$$

Error estimate on each sub-interval:

$$E_i(f; h) = \frac{1}{2} f''(\xi_i) \int_{x_i}^{x_{i+1}} (x - x_i) (x - x_{i+1}) dx = -\frac{1}{12} h^3 f''(\xi_i).$$

The total error is:

$$\begin{aligned} E(f; h) &= \sum_{i=0}^{n-1} E_i(f; h) = \sum_{i=0}^{n-1} -\frac{1}{12} h^3 f''(\xi_i) \\ &= -\frac{1}{12} h^3 \underbrace{\left[\sum_{i=0}^{n-1} f''(\xi_i) \right]}_{=f''(\xi)} \cdot \frac{1}{n} \cdot \underbrace{\frac{b-a}{h}}_n = n \end{aligned}$$

which gives

$$E(f; h) = -\frac{b-a}{12} h^2 f''(\xi), \quad \xi \in (a, b).$$

Error bound

$$|E(f; h)| \leq \frac{b-a}{12} h^2 \max_{x \in (a,b)} |f''(x)|$$

Simpson's rule

We now explore possibility of using higher order polynomials. We cut up $[a, b]$ into $2n$ equal sub-intervals

$$x_0 = a, \quad x_{2n} = b, \quad h = \frac{b-a}{2n}, \quad x_{i+1} - x_i = h$$

On $[x_{2i}, x_{2i+2}]$, interpolates $f(x)$ at the points $x_{2i}, x_{2i+1}, x_{2i+2}$ with a quadratic polynomial $p_i(x)$.

Lagrange form for $p_i(x)$:

$$\begin{aligned} p_i(x) &= f(x_{2i}) \frac{(x - x_{2i+1})(x - x_{2i+2})}{(x_{2i} - x_{2i+1})(x_{2i} - x_{2i+2})} + f(x_{2i+1}) \frac{(x - x_{2i})(x - x_{2i+2})}{(x_{2i+1} - x_{2i})(x_{2i+1} - x_{2i+2})} \\ &\quad + f(x_{2i+2}) \frac{(x - x_{2i})(x - x_{2i+1})}{(x_{2i+2} - x_{2i})(x_{2i+2} - x_{2i+1})} \end{aligned}$$

With uniform nodes, this becomes

$$p_i(x) = \frac{1}{2h^2} f(x_{2i}) (x - x_{2i+1}) (x - x_{2i+2}) - \frac{1}{h^2} f(x_{2i+1}) (x - x_{2i}) (x - x_{2i+2}) \\ + \frac{1}{2h^2} f(x_{2i+2}) (x - x_{2i}) (x - x_{2i+1})$$

We work out the integrals (try to fill in the details yourself!)

$$I_1 = \int_{x_{2i}}^{x_{2i+2}} (x - x_{2i+1}) (x - x_{2i+2}) dx = \frac{2}{3} h^3 \\ I_2 = \int_{x_{2i}}^{x_{2i+2}} - (x - x_{2i}) (x - x_{2i+2}) dx = \frac{4}{3} h^3 \\ I_3 = \int_{x_{2i}}^{x_{2i+2}} (x - x_{2i}) (x - x_{2i+1}) dx = \frac{2}{3} h^3$$

Then

$$\int_{x_{2i}}^{x_{2i+2}} p_i(x) dx = \frac{1}{2h^2} f(x_{2i}) \cdot I_1 + \frac{1}{h^2} f(x_{2i+1}) \cdot I_2 + \frac{1}{2h^2} f(x_{2i+2}) \cdot I_3 \\ = \frac{1}{2h^2} f(x_{2i}) \frac{2}{3} h^3 + \frac{1}{h^2} f(x_{2i+1}) \frac{4}{3} h^3 + \frac{1}{2h^2} f(x_{2i+2}) \frac{2}{3} h^3 \\ = \frac{h}{3} [f(x_{2i}) + 4f(x_{2i+1}) + f(x_{2i+2})].$$

We now sum them up

$$\int_a^b f(x) dx \approx S(f; h) = \sum_{i=0}^{n-1} \int_{x_{2i}}^{x_{2i+2}} p_i(x) dx \\ = \frac{h}{3} \sum_{i=0}^{n-1} [f(x_{2i}) + 4f(x_{2i+1}) + f(x_{2i+2})]$$

Simpson's Rule:

$$S(f; h) = \frac{h}{3} \left[f(x_0) + 4 \sum_{i=1}^n f(x_{2i-1}) + 2 \sum_{i=1}^{n-1} f(x_{2i}) + f(x_{2n}) \right]$$

$$\text{Simpson's Rule: } S(f; h) = \frac{h}{3} \left[f(x_0) + 4 \sum_{i=1}^n f(x_{2i-1}) + 2 \sum_{i=1}^{n-1} f(x_{2i}) + f(x_{2n}) \right]$$

```
In [ ]: import numpy as np

def f(x):
    return np.sqrt(x**2 + 1)

a = -2
b = 2
n = 10

h = (b - a) / (2 * n)
x = np.linspace(a, b, 2*n + 1)

S = (h / 3) * (f(x[0]) + 4 * np.sum(f(x[1:2*n:2])) + 2 * np.sum(f(x[2:2*n-1:2])) + f(x[2
```

S

Out[]: 5.915769549490477

```
In [ ]: import sympy as sp

# Define the symbol and the function
x = sp.symbols('x')
f = sp.sqrt(x**2 + 1)

# Calculate the integral
I = sp.integrate(f, (x, -2, 2))

I
```

Out[]: $\operatorname{asinh}(2) + 2\sqrt{5}$

```
In [ ]: I.evalf()
```

Out[]: 5.91577143017839

Error estimate for Simpson's Rule

The basic error on each sub-interval is

$$E_{S,i}(f; h) = -\frac{1}{90}h^5 f^{(4)}(\xi_i), \quad \xi_i \in (x_{2i}, x_{2i+2}).$$

(See lecture notes or textbook for the proof.) Then, the total error is

$$E_S(f; h) = I(f) - S(f; h) = -\frac{1}{90}h^5 \sum_{i=0}^{n-1} f^{(4)}(\xi_i) \frac{1}{n} \cdot \frac{b-a}{2h} = -\frac{b-a}{180}h^4 f^{(4)}(\xi),$$

This gives us the error bound

$$|E_S(f; h)| \leq \frac{b-a}{180}h^4 \max_{x \in (a,b)} |f^{(4)}(x)|.$$

Gaussian Quadrature

All the numerical integration rules follow the form

$$\int_a^b f(x)dx \approx A_0 f(x_0) + A_1 f(x_1) + \cdots + A_n f(x_n).$$

Here $x_i \in [a, b]$ are called the nodes, and A_i 's are the weights. For example, the trapezoid rule is:

$$x_0 = a, x_1 = b, A_0 = A_1 = \frac{b-a}{2}$$

and the Simpson's rule corresponds to

$$x_0 = a, x_1 = \frac{a+b}{2}, x_2 = b, A_0 = A_2 = (b-a)\frac{1}{6}, A_1 = (b-a)\frac{2}{3}.$$

In these rules, we fix the points x_i , then we adjust the weights A_i .

Idea: allow both the nodes x_i and the weights A_i to be adjusted, to achieve high accuracy.

One chooses the nodes x_i and weight $A_i (i = 0, 1, 2, \dots, N)$ such that the algorithm gives the exact value for polynomial functions $f(x)$ of highest possible degree m :

$$\int_a^b f(x)dx = A_0 f(x_0) + A_1 f(x_1) + \dots + A_n f(x_m), \quad \text{if } f \in P^m.$$

Here, m is called the degree of precision.

To fix the idea, we consider now the interval $[-1, 1]$. Start with $N = 1$, i.e., we have 2 nodes x_0, x_1 and 2 weights A_0, A_1 . The rule satisfies

$$\int_{-1}^1 f(x)dx = A_0 f(x_0) + A_1 f(x_1), \quad f \in \mathcal{P}_m$$

\Rightarrow the rule must be exact for functions $1, x, x^2, x^3, \dots, x^m$. We will need 4 equations for 4 unknowns, therefore $m = 3$. Recall that

$$\int_{-1}^1 x^k dx = \begin{cases} \frac{2}{k+1}, & k \text{ even} \\ 0, & k \text{ odd.} \end{cases}$$

$$\begin{aligned} f(x) = 1 : A_0 + A_1 &= 2 \\ f(x) = x : A_0 x_0 + A_1 x_1 &= 0 \\ f(x) = x^2 : A_0 x_0^2 + A_1 x_1^2 &= \frac{2}{3} \\ f(x) = x^3 : A_0 x_0^3 + A_1 x_1^3 &= 0 \end{aligned}$$

One could solve this system and find

$$x_0 = -\frac{1}{\sqrt{3}}, \quad x_1 = \frac{1}{\sqrt{3}}, \quad A_0 = 1, \quad A_1 = 1.$$

Then, we have the Gaussian quadrature rule for $n = 1$,

$$\int_{-1}^1 f(x)dx \approx f\left(-\frac{1}{\sqrt{3}}\right) + f\left(\frac{1}{\sqrt{3}}\right).$$

This will have degree of precision 3 .

Gaussian quadrature, $N = 2$ Nodes: x_0, x_1, x_2 , and weights: A_0, A_1, A_2 .

$$\int_{-1}^1 f(x)dx \approx A_0 f(x_0) + A_1 f(x_1) + A_2 f(x_2)$$

The rule should give exact solution for polynomials of degree $m = 5$. symmetry:

$$x_0 = -x_2, \quad x_1 = 0, \quad A_0 = A_2,$$

Only need to check with $f(x) = 1, x^2, x^4$:

$$f(x) = 1 : \quad 2A_0 + A_1 = 2$$

$$f(x) = x^2 : \quad 2A_0x_0^2 = 2/3$$

$$f(x) = x^4 : \quad 2A_0x_0^4 = 2/5$$

$$x_0 = \sqrt{3/5}, \quad x_1 = 0, \quad x_2 = -\sqrt{3/5}, \quad A_0 = A_2 = 5/9, \quad A_1 = 8/9.$$