APPLICATION: VOLTERRA INTEGRAL EQUATIONS

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Motivation

Physical Problems

2 Preliminaries

- Purpose of this talk
- Convolution Quadrature
- Fractional Linear Multistep Methods
 - Target Problem
 - Construction
 - Practicality
- 4 Convergence Analysis
 - Main result
 - Proof of the main result
- 5 Stability Analysis
 - Analytic Stability Regions
 - Stability Region of a Fractional Linear Multistep Method
 - Characterization of the Stability Region
 - Transformation of Stability Regions
 - Dahlquist Barrier for Fractional LMSMs

6 Numerical Experiments

• (BDF4)^{1/2}

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Numerical Experiments

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First appearance

Abel's Mechanical Problem

In the (x,y)-plane find a curve C which is the graph of an increasing function $x = \varphi(y), y \in [0, H]$, along which under constant downward acceleration g a particle must be constrained to fall, in order that its falling time equals a prescribed function t(y) of the initial height y.



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Abel's Mechanical Problem

In the absence of friction, the problem can be reduced to solving for φ in the equation

$$\int_0^y (y-z)^{-1/2} \sqrt{1+\varphi'(z)^2} \, \mathrm{d} z = \sqrt{2g} t(y).$$

Remark

The -1/2 exponent for the singular kernel often occurs for Abel Integral Equations arising from physics

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Shooting a particle at an atom nucleus

We are interested in determining the potential V(r) of the repelling field of an Atom nucleus. We can do so by measuring the angle of deflection θ a particle with impact parameter b > 0 experiences.



By impact parameter, we mean the closest distance the particle would approach the atom if it were to travel in a straight line.

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One can define a function for the angle of deflection θ by varying the impact parameter *b*, i.e. $\theta = \theta(b)$.

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One can define a function for the angle of deflection θ by varying the impact parameter *b*, i.e. $\theta = \theta(b)$.

$$\theta(b) = \pi - 2 \int_{r_0}^{\infty} \frac{\mathrm{d}r}{r^2 (b^{-2} - r^{-2} - E^{-1} b^{-2} V(r))^{1/2}}$$

where r_0 is the solution to

$$E - b^2 E r_0^{-2} - V(r_0) = 0$$

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A few change of variables later:

One can obtain an integral equation of the form

$$\beta(x) = \int_0^x \frac{g(w) \, \mathrm{d}w}{(x-w)^{1/2}}, \ 0 \le x \le \frac{1}{b_{\min}^2}.$$

Remark: The bound on the integral arises from the fact energy has been fixed.



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Previously in the Seminar

We have previously discussed the approximation of

$$(f\star g)(x)=\int_0^x f(s)g(x-s) \,\mathrm{d}s$$

- g is given explicitly. Only "scant" information about f is given (i.e. conditions suitable for the inversion of its Laplace transform)
- Obtained convolution quadratures from an appropriate linear multistep method(LMSM)
- Error analysis performed justified the use of convolution quadratures. In particular, the case $g(t) = t^{\alpha-1}$ was discussed

Convention

Unless otherwise stated, all LMSMs satisfy

- The method is stable and consistent of order p
- The method is implicit
- All zeros of $\sigma(\zeta)$ have absolute value ≤ 1 .

Purpose of this talk

We discuss a method for the numerical solution of a weakly singular Abel-Volterra integral equation

$$y(t) = f(t) + rac{1}{\Gamma(lpha)} \int_0^t (t-s)^{lpha-1} g(s,y(s)) \, \mathrm{d}s, \ \ 0 < lpha < 1 \ \mathrm{fixed}$$

How is this problem different?

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How is this problem different?

- We are approximating *y*! More precisely, we are *solving* the (nonlinear) integral equation numerically.
- Known quantities g and f (the latter not appearing in the integral).
- No information about the Laplace transform of y is assumed. Instead, we rely on a priori regularity and asymptotic properties.

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Definition

A suitable numerical scheme can be developed for a larger class of integral equations

Abel-Volterra Integral Equation of the Second Kind

$$y(t) = f(t) + \int_0^t K(t, s, y(s)) \, \mathrm{d}s$$

Remarks:

- Special case: $K(t,s,y(s)) = (t-s)^{\alpha-1}g(s,y(s)).$
- If K, f are independent of t, the equation reduces to the initial value problem

$$y' = K(t, y), y(0) = y_0.$$

Convolution Quadratures for the Abel-Volterra Integral Equation

We shall show a natural scheme to consider is of the form

$$y_n = f(x_n) + h \sum_{j=-1}^{-k} w_{nj} K(x_n, x_j, y_j) + h \sum_{j=0}^{n} \omega_{n-j} K(x_n, x_j, y_j) \ (n \ge 0)$$

where w_{nj} and ω_{n-j} are weights of (potentially) different methods

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where w_{nj} and ω_{n-j} are weights of (potentially) different methods Why is there an extra sum?!

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Applying LMSM to Abel-Volterra Integral Equation

Let (ρ, σ) be a LMSM.

Rewrite the Abel-Volterra equation

$$y(x) = J(x, x_n) + \int_{x_n}^{x} K(x, s, y(s)) ds, (x \ge x_n)$$

where $J(x, x_n) = f(x) + \int_0^{x_n} K(x, s, y(s)) \, ds$

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where $J(x, x_n) = f(x) + \int_0^{x_n} K(x, s, y(s)) ds$

Note: $y(x_n) = J(x_n, x_n)$

ODE Problem:

$$J(x,\xi) = f(x) + \int_0^\xi K(x,s,y(s)) \, \mathrm{d}s$$

Taking a partial derivative yields

$$\frac{\partial}{\partial\xi}J(x,\xi) = K(x,\xi,y(\xi)) \tag{1}$$

Approximation of $J_n = J(\cdot, x_n)$

Applying a LMSM to the ODE problem

Recall: k-step LMSMs require k initial values to "take-off"

Starting values y_{-k}, \ldots, y_{-1} are given. We assume the starting functions $\tilde{J}_{-k}, \ldots, \tilde{J}_{-1}$ are given by *some* quadrature (not necessarily related to (ρ, σ))

$$\tilde{J}_n(x) = f(x) + h \sum_{j=-1}^{-k} w_{nj} K(x, x_j, y_j) \ n \in \{-k, \dots, -1\}$$

Approximation of $J_n = J(\cdot, x_n)$

Applying a LMSM to the ODE problem

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Apply $(
ho,\sigma)$ to (1) and obtain an approximation $ilde{J}_n$ of J_n

$$\sum_{j=0}^{k} \alpha_{j} \tilde{J}_{n+j-k}(x) = h \sum_{j=0}^{k} \beta_{j} K(x, x_{n+j-k}, y_{n+j-k})$$
(2)

Set $y_n = \tilde{J}_n(x_n)$.

 y_n is an approximation of $y(x_n)$

Convolution Quadrature

Lemma

The LMSM (2) with starting functions(as above) can be rewritten as a quadrature method

$$y_n = f(x_n) + h \sum_{j=-1}^{-k} w_{nj} K(x_n, x_j, y_j) + h \sum_{j=0}^{n} \omega_{n-j} K(x_n, x_j, y_j) \ (n \ge 0)$$

where the weights ω_n and w_{nj} are bounded. The weights ω_n are the coefficients of the power series

$$\omega(\zeta) = rac{\sigma(\zeta^{-1})}{
ho(\zeta^{-1})}$$

Converse: If $\omega(\zeta)$ is a rational function, one can recover the LMSM

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Numerical Experiments

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Adapted Numerical Method for Convolution Type Kernels

We wish to apply a convolution quadrature to approximate

Abel-Volterra Integral Equation of the 2nd kind with a Convolution Kernel

$$y(t) = f(t) + \frac{1}{\Gamma(\alpha)} \int_0^t (t-s)^{\alpha-1} g(s, y(s)) \, \mathrm{d}s,$$

for $t \in [0, T]$ and $0 < \alpha < 1$ fixed.

Can we furnish a method adapted to this particular type of Abel-Volterra Integral Equation?

Idea: Consider fractional step-sizes and weights!

We seek to construct

Fractional Linear Multistep Method

$$y_n = f(t_n) + h^{lpha} \sum_{j=0}^m w_{nj}g(t_j, y_j) + h^{lpha} \sum_{j=0}^n \omega_{n-j}^{(lpha)}g(t_j, y_j)$$

- h > 0 denotes step-size
- $t_n = nh$
- starting quadrature weights w_{nj} (independent of h), j = 0, ..., m, with m fixed
- convolution quadrature weights $\omega_n^{(\alpha)}$

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$$y_n = f(t_n) + h^{\alpha} \sum_{j=0}^m w_{nj}g(t_j, y_j) + h^{\alpha} \sum_{j=0}^n \omega_{n-j}^{(\alpha)}g(t_j, y_j)$$

- h > 0 denotes step-size
- $t_n = nh$
- starting quadrature weights w_{nj} (independent of h), $j = 0, \ldots, m$, with m fixed
- convolution quadrature weights $\omega_n^{(\alpha)}$

Given (ρ, σ) , convolution quadrature weights $\omega_n^{(\alpha)}$ are obtained from the coefficients of the power series

$$\omega^{(\alpha)}(\zeta) = \left(\frac{\sigma(\zeta^{-1})}{\rho(\zeta^{-1})}\right)^{\alpha}$$

As a (non-trivial) consequence of our convention, $\omega_n^{(\alpha)} = O(n^{\alpha-1})$.

Pros:

- Efficient implementation
- Capture the nature of the equation

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But is this the *right* way to construct convolution quadratures?

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- Efficient implementation
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But is this the *right* way to construct convolution quadratures?

The Driving Question

Given a LMSM $\omega = (\rho, \sigma)$, can we construct a Convolution Quadrature satisfying

- same convergence properties as (ρ, σ)
- same stability properties as (ρ, σ)

Pros:

- Efficient implementation
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But is this the *right* way to construct convolution quadratures?

The Driving Question

Given a LMSM $\omega = (
ho, \sigma)$, can we construct a Convolution Quadrature satisfying

- same convergence properties as (ρ, σ)
- same stability properties as (ρ, σ)

The answer is yes!

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Convergence analysis setup

Consider

$$y(t) = f(t) + rac{1}{\Gamma(lpha)} \int_0^t (t-s)^{lpha-1} g(s,y(s)) \, \mathrm{d}s$$

Assume: g, f are sufficiently smooth

These conditions guarantee

- Uniqueness of solution y(t)
- Sufficient regularity of y(t)
- Our assertions are true

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Convergence result

Theorem

Given a LMSM $\omega = (\rho, \sigma)$, there exists a starting quadrature $w_{nj} = O(n^{\alpha-1})$ so that the error of the computed solution satisfies

$$|y_n-y(t)| \leq C \cdot t^{\beta-1} \cdot h^{\rho} \quad (t=nh \leq T),$$

for all *h* sufficiently small.

Remarks:

- C independent of n and h
- $\bullet \ \beta > \alpha$

Proof: Choosing the starting quadrature weights



For any sufficiently smooth function $\varphi(t)$, there exists a starting quadrature $w_{nj} = O(n^{\alpha-1})$ satisfying

$$h^{\alpha}\sum_{j=0}^{n}\omega_{n-j}^{(\alpha)}\varphi(jh)+h^{\alpha}\sum_{j=0}^{m}w_{nj}\varphi(jh)=\frac{1}{\Gamma(\alpha)}\int_{0}^{t}(t-s)^{\alpha-1}\varphi(s) \ \mathrm{d}s+O(t^{\beta-1}\cdot h^{p}),$$

for some $\beta > \alpha$. In particular,

$$egin{aligned} &h^lpha\sum_{j=0}^n\omega_{n-j}^{(lpha)}g(t_j,y(t_j))+h^lpha\sum_{j=0}^mw_{nj}g(t_j,y(t_j))\ &=rac{1}{\Gamma(lpha)}\int_0^t(t-s)^{lpha-1}g(s,y(s))\;\mathrm{d}s+O(t^{eta-1}\cdot h^
ho). \end{aligned}$$

Proof: Consistency Error

Define the *consistency error* at t = nh by

$$d_n = \left| h^{\alpha} \sum_{j=0}^n \omega_{n-j}^{(\alpha)} g(t_j, y(t_j)) + h^{\alpha} \sum_{j=0}^m \omega_{nj} g(t_j, y(t_j)) - \frac{1}{\Gamma(\alpha)} \int_0^t (t-s)^{\alpha-1} g(s, y(s)) \, \mathrm{d}s \right|$$

It follows

$$d_n \leq C \cdot n^{\beta-1} \cdot h^{p+\beta-1}$$

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Proof: Error Propagation The *global error* at t = nh is defined as

$$e_n = |y_n - y(t)|$$

Claim:

Bound on global error

$$e_n \leq C \cdot h^p \cdot t^{\beta-1}$$

Simplifying Assumption: *g* is Lipschitz continuous in the second argument. The triangle inequality yields

$$e_n \leq d_n + h^lpha L\left(\sum_{j=0}^n |\omega_{n-j}^{(lpha)}|e_j + \sum_{j=0}^m |w_{nj}|e_j
ight)$$

Recall, the weights are $O(n^{\alpha-1})$

Fact:

$$n^{\alpha-1} \leq (-1)^n \binom{-\alpha}{n},$$

where $(-1)^n \binom{-\alpha}{n}$ is the n-th coefficient of power series expansion of $(1-\zeta)^{-\alpha}$.

Proof: Error Propagation

Therefore, we can bound

$$e_n \leq C \cdot h^{p+eta-1} \cdot (-1)^n inom{-eta}{n} + h^lpha C \sum_{j=0}^n (-1)^{n-j} inom{-lpha}{n-j} e_j,$$

for some generic constant C > 0.

Hint: Try finding a power series $u(\zeta) = \sum_{j=0}^{\infty} u_n \zeta^n$ such that

 $e_n \leq C \cdot h^p \cdot u_n$

with (hopefully) $u_n = O(t^{\beta-1})$.

Proof: Error Propagation

Therefore, we can bound

$$e_n \leq C \cdot h^{p+eta-1} \cdot (-1)^n inom{-eta}{n} + h^lpha C \sum_{j=0}^n (-1)^{n-j} inom{-lpha}{n-j} e_j,$$

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Hint: Try finding a power series $u(\zeta) = \sum_{i=0}^{\infty} u_n \zeta^n$ such that

$$e_n \leq C \cdot h^p \cdot u_n$$

with (hopefully) $u_n = O(t^{\beta-1})$.

Fortunately, such a power series exists!

 $u(\zeta) = \frac{1}{h}V(\frac{1-\zeta}{h})$, where V(z) is the Laplace transform of

$$v(t) = \frac{t^{\beta-1}}{\Gamma(\beta)} + C \int_0^t \frac{(t-s)^{\alpha-1}}{\Gamma(\alpha)} v(s) \, \mathrm{d}s.$$

works. This completes the proof.

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Numerical Experiments (BDF4)^{1/2}

Analytic stability region of the Abel-Volterra Integral Equation

For this discussion, we consider a linearized Abel-Volterra integral equation

$$y(t) = f(t) + rac{\lambda}{\Gamma(lpha)} \int_0^t (t-s)^{lpha-1} y(s) \, \mathrm{d}s, \ t \ge 0, 0 < lpha < 1$$

Stability Theorem

- If $|\arg \lambda \pi| < (1 \alpha/2)\pi$, the solution y(t) satisfies
 - $y(t) \rightarrow 0$ as $t \rightarrow \infty$ whenever f(t) converges to a finite limit
 - y(t) is bounded whenever f(t) is bounded.

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Stability region of a Fractional LMSM

Apply fractional LMSM

$$y_n = f_n + h^{\alpha} \lambda \sum_{j=0}^n \omega_{n-j}^{(\alpha)} y_j,$$

where $f_n = f(t_n) + h^{\alpha} \lambda \sum_{i=0}^{m} w_{ni} y_i$

Stability Region of a Fractional LMSM

$$S = \{\lambda \in \mathbb{C} : f_n \to L \text{ implies } y_n \to 0\}$$

Stability Preservation

Since $w_{ni} = O(n^{\alpha-1})$, it follows that $\lim_{n\to\infty} f_n = L$ whenever $\lim_{t\to\infty} f(t) = L$. If $f_n \to L$ implies $y_n \rightarrow 0$, then the stability region should at least contain the analytic stability region

- If $\{z \in \mathbb{C} : |\arg z \lambda| < (1 \alpha/2)\pi\} \subset S$ the method is A-stable
- If $\{z \in \mathbb{C} : |\arg z \pi| < \varphi\} \subset S$, the method is $A(\varphi)$ -stable.

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Example 1: Stability region of an A-stable Fractional LMSM Contains the *red* wedge



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Characterization of the Stability Region

Recall: Stability region for a LMSM is given by

 $S = \mathbb{C} \setminus \{
ho(\zeta) / \sigma(\zeta) : \ |\zeta| \ge 1 \} = \mathbb{C} \setminus \{ 1 / \omega(\zeta) : \ |\zeta| \le 1 \}$

A similar characterization for Fractional LMSMs exists

Theorem

The stability region of a fractional LMSM is given by

 $S = \mathbb{C} \setminus \{1/\omega^{(\alpha)}(\zeta) : |\zeta| \le 1\}.$

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Transformation of Stability Regions

Corollary

Let $\omega = (\rho, \sigma)$ and ω^{α} its corresponding fractional LMSM. Letting $S_{\omega}, S_{\omega^{\alpha}}$ denote their respective stability regions, we have:

- (a) $(\mathbb{C} \setminus S_{\omega^{\alpha}}) = (\mathbb{C} \setminus S_{\omega})^{\alpha}$
- (b) ω^{α} is A-stable if and only if ω is A-stable
- (c) With $\pi \varphi = \alpha(\pi \psi)$, ω^{α} is $A(\varphi)$ -stable if and only if ω is $A(\psi)$ -stable

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Example 2: Stability region of an $A(\psi)$ -stable FLMSM

Suppose $\omega = (\rho, \sigma)$ is $A(\varphi)$ -stable, i.e. its stability region contains the *red* wedge



Example 2: Stability region of an $A(\psi)$ -stable FLMSM

For $0 < \alpha \ll 1$, ω^{α} is $A(\psi)$ -stable, so its stability region contains the *red* wedge



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Example 2: Stability region of an $A(\psi)$ -stable FLMSM

Or $0 \ll \alpha < 1 \ \omega^{\alpha}$ is $A(\psi)$ -stable, so its stability region contains the *red* wedge



Consistency

Fractional LMSMs consistent of order p satisfy

$$h^{\alpha}\omega^{\alpha}(e^{-h}) = 1 + \alpha c^* h^p + O(h^{p+1})$$

c* is referred to as the error constant

Theorem

The order of an A-stable fractional linear multistep method cannot exceed 2.

Example: Fractional Trapezoidal Rule The fractional trapezoidal rule, defined by

$$\omega^lpha(\zeta) = \left(rac{1+\zeta}{2-2\zeta}
ight)^lpha$$

is A-stable and has order 2. In particular, it achieves the smallest error constant, $c^{*}=1/12.$

A Proof from First Principles

An A-stable fractional method satisfies

$$|rg \omega^lpha(\zeta)| \leq rac{lpha}{2} \pi, \; |\zeta| \leq 1, \; \zeta
eq 1.$$

Complexify $h^{\alpha}\omega^{\alpha}(e^{-h}) - 1$ i.e. consider the function $z^{\alpha}\omega^{\alpha}(e^{-z}) - 1$.

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Observe:

- For $z \in (0, i\pi]$, $\operatorname{Im}[z^{\alpha}\omega^{\alpha}(e^{-z})] \geq 0$
- For both $z \in \mathbb{R}^+$ and $z \in i\pi + \mathbb{R}^+$, $\operatorname{Im}[z^{\alpha}\omega^{\alpha}(e^{-z})] \ge 0$ $\omega^{\alpha}(e^{-z}) = \omega^{\alpha}(0) + O(e^{-\operatorname{Re}z})$, for sufficiently large Rez. and $\omega^{\alpha}(0) > 0$



A Proof from First Principles

Therefore

 $\operatorname{Im}[z^{lpha}\omega^{lpha}(e^{-z})]\geq 0$ orall z on the boundary of the rectangle

Maximum Principle implies

 $\text{Im}[z^{\alpha}\omega^{\alpha}(e^{-z})] \ge 0 \ \forall z \text{ in the interior of the rectangle}$

Consistency of order *p* gives

 $0 \leq \operatorname{Im}[z^{\alpha}\omega^{\alpha}(e^{-z}) - 1] = \alpha c^* \operatorname{Im} z^{\rho} + O(z^{\rho})$

which holds for $z \rightarrow 0$ and $0 \leq \arg z \leq \pi/2$.

This can only happen if $p \leq 2$.

Motivation

• Physical Problems

2 Preliminaries

- Purpose of this talk
- Convolution Quadrature
- Fractional Linear Multistep Methods
 - Target Problem
 - Construction
 - Practicality

4 Convergence Analysis

- Main result
- Proof of the main result

5 Stability Analysis

- Analytic Stability Regions
- Stability Region of a Fractional Linear Multistep Method
- Characterization of the Stability Region
- Transformation of Stability Regions
- Dahlquist Barrier for Fractional LMSMs

6 Numerical Experiments

• (BDF4)^{1/2}

 $(BDF4)^{1/2}$

Consider the integral equation

$$y(t) = -\frac{1}{\sqrt{\pi}} \int_0^t (t-s)^{-1/2} (y(s) - \sin s)^3 \, \mathrm{d}s.$$

Convolution quadrature weights generated by

$$\omega^{1/2}(\zeta) = \left(\frac{25}{12} - 4\zeta + 4\zeta^2 - \frac{4}{3}\zeta^3 + \frac{1}{4}\zeta^4\right)^{-\frac{1}{2}}$$

Exact solution y(8) = 0.3236412904 is known.

h	numerical solution	error	error/h ⁴
0.1	0.3236520328	$1.07 imes10^{-5}$	0.107
0.05	0.3236421096	$8.19 imes10^{-7}$	0.1314
0.025	0.3236413206	$3.02 imes 10^{-8}$	0.0773

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