

Convolution Quadrature and Discretized Operational Calculus. I.

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Summary. Numerical methods are derived for problems in integral equations (Volterra, Wiener-Hopf equations) and numerical integration (singular integrands, multiple time-scale convolution). The basic tool of this theory is the numerical approximation of convolution integrals

$$f * g(x) = \int_{0}^{x} f(x-t) g(t) dt \qquad (x \ge 0)$$

by convolution quadrature rules. Here approximations to f * g(x) on the grid x = 0, h, 2h, ..., Nh are obtained from a discrete convolution with the values of g on the same grid. The quadrature weights are determined with the help of the Laplace transform of f and a linear multistep method. It is proved that the convolution quadrature method is convergent of the order of the underlying multistep method.

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1. Introduction

1.1. Derivation of the Methods

We begin our investigations with the numerical approximation of convolution integrals

$$\int_{0}^{\infty} f(t) g(x-t) dt \quad (x \ge 0).$$
(1.1)

We shall obtain methods of discrete convolution form

$$\sum_{0 \le jh \le x} \omega_j(h) g(x-jh)$$
(1.2)

where h > 0 is the stepsize, and the quadrature weights $\omega_j(h)$ are the coefficients of the power series

$$F(\delta(\zeta)/h) = \sum_{j=0}^{\infty} \omega_j(h)\zeta^j.$$
 (1.3)

Here F is the Laplace transform of f, and $\delta(\zeta) = \sum_{0}^{\infty} \delta_j \zeta^j$ is the quotient of the

generating polynomials of a linear multistep method.

As will be pointed out in Part II of this work, quadrature methods of this type are particularly suited to the approximation of convolution integrals whose kernel f(t) is singular or has components at different time-scales; to the numerical evaluation of the expressions arising in classical operational calculus where the Laplace transform F of the convolution kernel (and not the kernel f itself) is known a priori; and to obtain stable discretizations of integral equations. From the control engineer's viewpoint our results can be seen as results on the discrete-time simulation of a continuous-time linear system given via its transfer function F(s).

To explain this approach we start from the Laplace inversion formula

$$f(t) = \frac{1}{2\pi i} \int_{\Gamma} F(\lambda) e^{\lambda t} d\lambda \qquad (t > 0)$$
(1.4)

which holds if, for example, we assume

 $F(s) \text{ is analytic in a sector } |\arg(s-c)| < \pi - \varphi \text{ with } \varphi < \frac{\pi}{2}, c \in \mathbb{R} \text{ and satisfies there}$ $|F(s)| \le M \cdot |s|^{-\mu} \text{ for some } M < \infty, \mu > 0.$ (1.5)

The contour Γ can then be chosen as running from $\infty \cdot e^{-i(\pi-\varphi)}$ to $\infty \cdot e^{i(\pi-\varphi)}$ within the sector of analyticity of F(s). A condition equivalent to (1.5) is that f(t) is analytic and of (at most) exponential growth in a sector containing the positive real half-line and satisfies $f(t) = O(t^{\mu-1})$ as $t \to 0$ within the sector. The assumption $\mu > 0$ guarantees in particular that f(t) is locally integrable. Examples include fractional powers, logarithms and most special functions.

The approach (1.2), (1.3) now comes about in the following way: Inserting (1.4) into (1.1) and reversing the order of integration gives

$$\int_{0}^{x} f(t) g(x-t) dt = \frac{1}{2\pi i} \int_{\Gamma} F(\lambda) \int_{0}^{x} e^{\lambda t} g(x-t) dt d\lambda.$$
(1.6)

We now approximate the inner integral by applying a linear multistep method to the differential equation $y' = \lambda y + g$, y(0) = 0,

$$\sum_{j=0}^{k} \alpha_{j} y_{n+j-k} = h \sum_{j=0}^{k} \beta_{j} (\lambda y_{n+j-k} + g((n+j-k)h)) \quad (n \ge 0),$$
(1.7)

with starting values $y_{-k} = ... = y_{-1} = 0$, and with $g \in C[0, \infty)$ extended by 0 to the negative real axis. Multiplying (1.7) by ζ^n and summing over *n* from 0 to ∞ we obtain

$$(\alpha_0 \zeta^k + \ldots + \alpha_k) \cdot \mathbf{y}(\zeta) = (\beta_0 \zeta^k + \ldots + \beta_k) \cdot (h \lambda \cdot \mathbf{y}(\zeta) + h \cdot \mathbf{g}(\zeta)),$$

with the generating (formal) power series $\mathbf{y}(\zeta) = \sum_{0}^{\infty} y_n \zeta^n$, $\mathbf{g}(\zeta) = \sum_{0}^{\infty} g(nh) \zeta^n$. Solving

this equation for $\mathbf{y}(\zeta)$ we find that y_n is the *n*-th coefficient of the power series $(\delta(\zeta)/h - \lambda)^{-1} \mathbf{g}(\zeta)$, where

$$\delta(\zeta) = (\alpha_0 \zeta^k + \ldots + \alpha_{k-1} \zeta + \alpha_k)/(\beta_0 \zeta^k + \ldots + \beta_{k-1} \zeta + \beta_k).$$
(1.8)

Hence the resulting approximation of (1.6) at x = nh is the *n*-th coefficient of

$$\frac{1}{2\pi i} \int_{\Gamma} F(\lambda) \left(\frac{\delta(\zeta)}{h} - \lambda \right)^{-1} \mathbf{g}(\zeta) \, d\lambda = F\left(\frac{\delta(\zeta)}{h} \right) \mathbf{g}(\zeta) \tag{1.9}$$

where the equality holds by Cauchy's integral formula. The coefficients of the right-hand side of (1.9) are the Cauchy product of the two sequences $\{\omega_j(h)\}$ of (1.3) and $\{g(jh)\}$. This gives finally (1.2).

The above derivation indicates also how to obtain error estimates: One studies first the error introduced by approximating the inner integral in (1.6) by the multistep method (1.7), then multiplies the obtained error bound by the bound (1.5) of $F(\lambda)$ and integrates along the contour Γ . This will actually be carried out in Sects. 2 and 3.

Of the linear multistep method we shall assume that it is $A(\alpha)$ -stable with $\alpha > \varphi$ of (1.5), stable in a neighbourhood of infinity, strongly zero-stable and consistent of order p. In terms of $\delta(\zeta)$, these conditions can be expressed as:

 $\delta(\zeta)$ is analytic and without zeros in a neighbourhood of the closed unit disc $|\zeta| \leq 1$, with the exception of a zero at $\zeta = 1$. (1.10a)

$$|\arg \delta(\zeta)| \leq \pi - \alpha$$
 for $|\zeta| < 1$, for some $\alpha > \varphi$. (1.10b)

$$\frac{1}{h}\delta(e^{-h}) = 1 + O(h^p) \quad \text{for some } p \ge 1.$$
(1.10c)

Well-known examples are the backward differentiation formulas of order $p \le 6$, given by $\delta(\zeta) = \sum_{i=1}^{p} \frac{1}{i} (1-\zeta)^{i}$, with $\alpha = 90^{\circ}$, 90°, 88°, 73°, 51°, 18° for p = 1, ..., 6, respectively.

Condition (1.5) on the *transfer function* (or *symbol*) F(s) of the convolution (1.1), and condition (1.10) on the discretization method will serve as the main assumption for all results of this paper.

Remark. (1.3) is well-defined if δ_0/h is in the domain of analyticity of F(s). Since $\delta_0 > 0$ by (1.10), this is satisfied at least for sufficiently small h > 0. The integrals in (1.6) and (1.9) are absolutely convergent, because $\mu > 0$ in (1.5).

1.2. Symbolic Notation and Historical Remarks

It will be convenient to use transfer function notation for the convolution (1.1),

$$F(s) g(x) = f * g(x) = \int_{0}^{x} f(t) g(x-t) dt \quad (s: \text{ complex variable}).$$
(1.11)

We use the abbreviation $s_h = \delta(\zeta)/h$ and employ discrete transfer function notation for (1.2), (1.3),

$$F(s_h) g(x) = \sum_{\substack{0 \le jh \le x}} \omega_j(h) g(x-jh).$$
(1.12)

(Note that $F(s_h) = \sum_{0}^{\infty} \omega_j(h) \zeta^j$ is the discrete Laplace transform of the sequence $\{\omega_j(h)\}$.)

With this notation we obtain from (1.9) the "Cauchy integral formula"

$$F(s_h) g(x) = \frac{1}{2\pi i} \int_{\Gamma} F(\lambda) \cdot (s_h - \lambda)^{-1} g(x) \cdot d\lambda, \qquad (1.13)$$

and the same relation, with s formally in place of s_h , holds by (1.6), since $(s - \lambda)^{-1}$ is the Laplace transform of $e^{\lambda t}$.

We shall use the notation (1.11) also for distributional convolution, in particular for differentiation

$$sg = \delta' * g = g' + g(0) \cdot \delta$$
 (Dirac's δ). (1.14)

As usual, we identify distributions with functions outside their singular support (which will be at most $\{0\}$ in our applications), so that (sg)(x) = g'(x) for x > 0. The derivative (1.14) is discretized by the backward difference approximation

$$s_h g(x) = \frac{1}{h} \sum_{0 \le jh \le x} \delta_j g(x-jh).$$
 (1.15)

With this in mind, the discretization process leading from (1.11) to (1.12) has a simple interpretation: The symbol of differentiation, s, is replaced by the symbol of a backward difference quotient, s_h . This idea of a discretized operational calculus has actually very old origins and seems to have been rediscovered several times. Of particular historical interest in this context is the work of Post [12] who has shown pointwise convergence of $F(s_h) g(x)$ as $h \to 0$ for the simple difference quotient $s_h g(x) = (g(x) - g(x-h))/h$, thereby generalizing earlier work of Liouville [10] and Grünwald [8] on fractional integrals, i.e. the case $F(s) = s^{-\mu}$. Post's work appears to have gone unnoticed in numerical analysis (in which he himself showed no interest), and the author of the present paper is not aware of any results in the literature going beyond those of Post.

1.3. Outline of the Paper

In Sect. 2 we study the convergence properties of the linear multistep method (1.7) (i.e., of $(s_h - \lambda)^{-1} g(x)$) for λ varying in a sector of the complex left half-plane. Such problems have previously been studied in the numerical analysis of parabolic differential equations by Zlámal [15] and Crouzeix and Raviart [2], see also Gekeler [7]. Here we give (and require) stronger estimates in terms of the input g, using different techniques.

Section 3 contains the first main results. The convergence properties of convolution quadrature rules $F(s_h) g(x)$ are now immediately obtained by integrating the error bounds of Sect. 2 along the contour Γ . The convergence order of the underlying multistep method, p, is obtained for $g \in C^p[0, \infty)$ by adding a few correction terms to $F(s_h) g(x)$,

$$F(s_h)^{\sim} g(x) = F(s_h) g(x) + \sum_{j=0}^{p-2} w_{nj}(h) g(jh)$$
 at $x = nh.$ (1.16)

These are required because of the special choice of starting values in (1.7), unless g near 0 or f near x = nh is "small".

In Sect. 4 we turn our attention to the coefficients $\omega_n(h)$ of (1.3) themselves, or rather to $f_n(h) = \omega_n(h)/h$ which is shown to approximate the inverse Laplace transform f(t) of F(s) at t = nh (away from 0) with the full order of the multistep method (1.7). This result (which comes rather unexpected) extends the classical Post-Widder inversion formula. Its numerical importance is perhaps not so much in the numerical inversion of Laplace transforms, but in the fact that it justifies replacing the weights $\omega_n(h)$ by hf(nh) for nh bounded away from 0, and in a very simple choice of the starting weights $w_{ni}(h)$ of (1.16).

In Sect. 5 we give some extensions of the results in Sect. 3. These concern the approximation of derivatives

$$\left(\frac{d}{dx}\right)^k \int_0^x f(t) g(x-t) dt \qquad (x>0)$$

("finite part integrals") and the convergence of (1.2) under weakened smoothness assumptions on g, in particular for the important case $g(t) = t^{\beta-1} \tilde{g}(t)$ with $\beta > 0$, \tilde{g} smooth, for which p-th order convergence can again be preserved by a modification of the form (1.16).

Topics which have been omitted are an extension to the non-sectorial, "hyperbolic" case, where F(s) is analytic and suitably bounded only in some half-plane Re s > c. For A-stable linear multistep methods (1.7) one can still obtain convergence results (of order at most 2, according to Dahlquist's [4] well-known order barrier.) Another omission concerns convolution quadratures

in which the underlying multistep method is the trapezoidal rule, $s_h = \frac{2}{h}$ (1)

 $-\zeta$ /(1+ ζ), which does not satisfy (1.10a). It appears, however, in the control literature where it is known as Tustin's method (after Tustin [13]; see, e.g., Franklin and Powell [6]).

2. Linear Multistep Methods Applied to $y' = \lambda y + g$ with λ Varying in a Sector

In this section we derive some technical estimates which will be required for the subsequent development. We begin with some preparation.

Since $F(s_h)g$ is the convolution of g with the sequence $\{\omega_n(h)\}_0^\infty$, the associativity of convolution yields

$$F(s_h)(g_1 * g_2) = (F(s_h)g_1) * g_2, \qquad (2.1)$$

and similarly

$$F(s)(g_1 * g_2) = (F(s)g_1) * g_2.$$
(2.2)

We shall use these relations in place of the usual Peano kernel technique. They permit to reduce the study of the error $F(s_h) g(x) - F(s) g(x)$ to the polynomial case $g(x) = x^q$, since

$$g(x) = \sum_{q=0}^{p-1} \frac{g^{(q)}(0)}{q!} x^{q} + \frac{1}{(p-1)!} (t^{p-1} * g^{(p)})(x), \qquad (2.3)$$

the Taylor expansion of g at 0.

Here we have denoted by t^{p-1} the function $t \mapsto t^{p-1}$ on $[0, \infty)$, and the same notation will also be used for other exponents in the following.

We now study the error of $(s_h - \lambda)^{-1} g(x)$, i.e., of the linear multistep method (1.7).

Lemma 2.1. Let $s_h = \delta(\zeta)/h$ satisfy (1.10).

a) For $|\arg(-\lambda)| \leq \alpha' < \alpha$ and $|h\lambda| \geq r > 0$ we have

$$|(s_h - \lambda)^{-1} t^q(x) - (s - \lambda)^{-1} t^q(x)| \leq \frac{C}{|h\lambda|} \cdot \rho^{x/h} \cdot \frac{h^q}{|\lambda|} \quad (q = 0, 1, ..., p)$$

with C = C(r) and $\rho = \rho(r) < 1$ independent of $h \in (0, 1]$, $x \ge h$ and λ .

b) To arbitrary $0 < \kappa < 1$ there exists $r_0 > 0$ such that for $|\arg(-\lambda)| \le \alpha' < \frac{\pi}{2}$ and $|h\lambda| \le r_0$

$$|(s_{h}-\lambda)^{-1} t^{q}(x) - (s-\lambda)^{-1} t^{q}(x)| \leq \begin{cases} C \cdot |e^{\kappa \lambda x}| \cdot h^{q+1} & (q=0, 1, \dots, p-1) \\ C \cdot |e^{\kappa \lambda x}| \cdot \frac{h^{p}}{|\lambda|} & (q=p) \end{cases}$$

with C independent of $h \in (0, 1]$, $x \ge 0$ and λ .

Remark. Except for q=0 the estimate in a) holds also for $0 \le x < h$. (In this interval $F(s_h) g(x) = F(\delta_0/h) \cdot g(x)$, and error estimates are easily derived.)

It is easily verified that

$$(s_h - \lambda)^{-1} g(x) - (s - \lambda)^{-1} g(x) = -(s_h - \lambda)^{-1} (s_h y - y')(x)$$
(2.4)

where $y = (s - \lambda)^{-1}g$, the solution of $y' = \lambda y + g$, y(0) = 0. We study $s_h y - y'$ in Lemma 2.2 (consistency), and $(s_h - \lambda)^{-1}$ in Lemma 2.3 (stability). Lemma 2.1 is derived from these estimates without new difficulty.

Lemma 2.2. a) For
$$|\arg(-\lambda)| \leq \alpha' < \frac{\pi}{2}$$
 and $|h\lambda| \geq r > 0$ we have

$$|(s_h - s)(s - \lambda)^{-1} t^q(x)| \le \frac{C}{|h\lambda|} \cdot \rho^{x/h} \cdot h^q \quad (q = 0, 1, ..., p)$$

with C = C(r) and $\rho = \rho(r) < 1$ independent of $h \in (0, 1]$, $x \ge h$ and λ .

b) There exists r > 0 such that for $|h\lambda| \leq r$

$$|(s_h - s)(s - \lambda)^{-1} t^q(x)| \leq C_1 \cdot |\lambda^{p-q} e^{\lambda x}| \cdot h^p + C_2 \cdot \rho^{x/h} \cdot h^q \qquad (q = 0, 1, ..., p)$$

with C_1 , C_2 and $\rho < 1$ independent of $h \in (0, 1]$, $x \ge 0$ and λ . Proof. First we show that

$$(s_h - s) t^q(x) | \leq C \cdot \rho^{x/h} \cdot h^{q-1} \qquad (q = 0, 1, \dots, p)$$
 (2.5)

with C and $\rho < 1$ independent of h and x > 0.

Taylor expansion in (1.10c) shows (cf. Lemma 5.3 of Henrici [9]) that

$$\frac{1}{h}\sum_{j=0}^{\infty}\delta_j(x-jh)^q = q \cdot x^{q-1} \quad \text{for } q=0, 1, \dots, p, \quad \text{for all } h \text{ and } x.$$

By (1.10a), $\delta_j = O(\rho^j)$ for some $\rho < 1$. Let now $x = nh + \theta h$ with $0 \le \theta < 1$. Then

$$|(s_{h}-s)t^{q}(x)| = \left|\frac{1}{h}\sum_{j=0}^{n}\delta_{j}(x-jh)^{q}-q\cdot x^{q-1}\right|$$

= $\frac{1}{h}\left|\sum_{j=n+1}^{\infty}\delta_{j}(x-jh)^{q}\right| \le h^{q-1}\sum_{j=1}^{\infty}|\delta_{n+j}|j^{q} \le C\cdot h^{q-1}\cdot\rho^{n}\left(\sum_{j=1}^{\infty}\rho^{j}j^{q}\right).$

This proves (2.5).

a) By (2.1) and (2.2),

$$(s_h - s)(s - \lambda)^{-1} t^q = (s_h - s)(e^{\lambda t} * t^q) = e^{\lambda t} * (s_h - s) t^q.$$

For $\tilde{\rho} = e^{-\tilde{\gamma}}$ with $\tilde{\rho} \ge \rho$ the estimate (2.5) yields thus

$$|(s_h-s)(s-\lambda)^{-1}t^q(x)| \leq C \cdot h^{q-1} \cdot e^{-\tilde{\gamma}x/h} \int_0^x e^{t[\operatorname{Re}(h\lambda)+\tilde{\gamma}]/h} dt.$$

(For q=0 there appears an additional term $|e^{\lambda x}|$ on the right-hand side of this estimate, caused by $s1 = \delta$ (Dirac's δ). For $x \ge h$ this term does, however, not affect the final estimate, and is therefore omitted in the following.) Fix

now r > 0. We can choose $\tilde{\gamma} = \tilde{\gamma}(r) > 0$ such that

$$\operatorname{Re}(h\lambda)+\tilde{\gamma}<-c<0\quad \text{ for } |\operatorname{arg}(-\lambda)|\leq \alpha'<\frac{\pi}{2}, \quad |h\lambda|\geq r.$$

Then the upper limit of the above integral can be extended to infinity, and we obtain the estimate

$$|(s_h - s)(s - \lambda)^{-1} t^q(x)| \leq \frac{C \cdot h}{-\left[\operatorname{Re}(h\lambda) + \tilde{\gamma}\right]} \cdot e^{-\tilde{\gamma}x/h} \cdot h^{q-1} \leq \frac{\tilde{C}}{|h\lambda|} \cdot \tilde{\rho}^{x/h} \cdot h^q.$$

This gives a).

b) By partial integration,

$$\frac{1}{q!}(s-\lambda)^{-1}t^{q} = \frac{t^{q}}{q!} * e^{\lambda t} = \frac{t^{q+1}}{(q+1)!} + \lambda \frac{t^{q+2}}{(q+2)!} + \dots + \lambda^{p-q-1} \frac{t^{p}}{p!} + \lambda^{p-q} \frac{t^{p}}{p!} * e^{\lambda t}.$$

Using (2.5) with q + 1, ..., p instead of q we obtain thus for $|h\lambda| \leq \text{const.}$

$$|(s_{h}-s)(s-\lambda)^{-1}t^{q}(x)| \leq C_{2} \cdot \rho^{x/h} \cdot h^{q} + C_{1} \cdot |\lambda^{p-q}| \cdot h^{p-1} \cdot (\rho^{t/h} * |e^{\lambda t}|)(x).$$
(2.6)

Let now $\rho = e^{-\gamma}$ and choose r > 0 so small that

$$\operatorname{Re}(h\lambda) + \gamma > c > 0 \quad \text{for } |h\lambda| \leq r.$$

Then

$$(\rho^{t/h} * |e^{\lambda t}|)(x) = |e^{\lambda x}| \cdot \int_{0}^{x} e^{-t [\operatorname{Re}(h\lambda) + \gamma]/h} dt \leq \frac{h}{c} |e^{\lambda x}|.$$

Inserting this estimate in (2.6) yields the result. \Box

We have $(s_h - \lambda)^{-1} = h(\delta(\zeta) - h\lambda)^{-1}$. For the coefficients of this power series we have the following stability estimate.

Lemma 2.3. a) For $|\arg(-z)| \leq \alpha' < \alpha$ and $|z| \geq r > 0$ the power series $(\delta(\zeta) - z)^{-1}$ is majorized by $\frac{M}{|z|} \sum_{0}^{\infty} \rho^n \zeta^n$ with M = M(r) and $\rho = \rho(r) < 1$ independent of z.

b) Let $0 < \kappa < 1$. There exists $r = r(\kappa) > 0$ such that for $|\arg(-z)| \le \alpha' < \frac{\pi}{2}$ and $|z| \le r$ the series $(\delta(\zeta) - z)^{-1}$ is majorized by $M \cdot \sum_{0}^{\infty} |e^{n\kappa z}| \zeta^n$ with M independent of z.

Proof. a) By (1.10) the series $\delta(\zeta) - z$ is for $|z| \ge r$, $|\arg(-z)| \le \alpha' < \alpha$ analytic and without zeros in a disc $|\zeta| \le 1/\rho$ with $\rho < 1$, where ρ is independent of z (but depends on r). Also

$$\sup_{|\zeta| \leq 1/\rho} |(\delta(\zeta) - z)^{-1}| \leq \frac{M}{|z|}$$

with $M < \infty$ independent of z. Hence Cauchy's estimate (e.g. Ahlfors [1, p. 98]) yields that the *n*-th coefficient of $(\delta(\zeta) - z)^{-1}$ is bounded by $M \rho^n / |z|$. This gives a).

b) Since $\delta(1)=0$, the estimates in a) deteriorate as $r \to 0$. For small |z| we use instead (1.10c). We define R(z) implicitly by

$$\delta(1/R(z)) = z, \quad R(0) = 1.$$
 (2.7)

We split

$$\frac{1}{\delta(\zeta)-z} = \frac{1-R(z)\zeta}{\delta(\zeta)-z} \cdot \frac{1}{1-R(z)\zeta}.$$

From (1.10c) we obtain

$$R(z) = e^z + O(z^{p+1}).$$

Hence there exists $r = r(\kappa) > 0$ such that

$$\left|\frac{R(z)}{e^{\kappa z}}\right| = |e^{(1-\kappa)z} + O(z^{p+1})| = |1 + (1-\kappa)z + O(z^2)| \le 1$$

for $|z| \leq r$ and $|\arg(-z)| \leq \alpha' < \frac{\pi}{2}$. Therefore

$$\frac{1}{1-R(z)\zeta} \quad \text{is majorized by} \quad \frac{1}{1-|e^{\kappa z}|\zeta}$$

On the other hand, using (1.10a) Cauchy's estimate yields

$$\frac{1-R(z)\zeta}{\delta(\zeta)-z} \quad \text{is majorized by} \quad \frac{M}{1-\rho\zeta},$$

with M and $\rho < 1$ independent of z. Hence

$$\frac{1}{\delta(\zeta)-z}$$
 is majorized by $\frac{M}{1-\rho\zeta} \cdot \frac{1}{1-|e^{\kappa z}|\zeta}$.

We can choose r so small that $e^{\kappa r} \rho < 1$. For the *n*-th coefficient of the above series we then obtain

$$\sum_{j=0}^{n} \rho^{j} |e^{\kappa z}|^{n-j} \leq |e^{\kappa z}|^{n} \sum_{j=0}^{\infty} \rho^{j} |e^{\kappa z}|^{-j} \leq |e^{\kappa z}|^{n} \frac{1}{1 - \rho e^{\kappa r}}.$$

This proves b). \Box

3. Convergence of Operational Quadratures

We are now in a position to show convergence of $F(s_h) g(x)$.

Theorem 3.1. Under the assumptions (1.5), (1.10) we have

$$|F(s_h)g(x) - F(s)g(x)| \leq C \cdot x^{\mu^{-1}} \cdot \{h | g(0)| + \dots + h^{p^{-1}} | g^{(p^{-2})}(0)| + h^p \cdot (|g^{(p^{-1})}(0)| + x \cdot \max_{0 \leq t \leq x} |g^{(p)}(t)|) \}$$

where the constant C does not depend on $h \in (0, \bar{h}]$, $x \in [h, \bar{x}]$ with fixed $\bar{x} < \infty$, and $g \in C^p[0, \bar{x}]$.

Remark. If additionally F(s) is exponentially stable (i.e., F(s) is analytic in some half-plane Re $s > \gamma$ with negative γ), Theorem 3.1 extends to a result of uniform convergence on the half-line $x \ge 1$, with exponential decay in the low-order error terms caused by $g(0), \ldots, g^{(p-2)}(0)$. (The proof is even slightly simpler, since no contour-shifting is necessary on intervals bounded away from 0.)

Proof. By (2.1)-(2.3),

$$F(s_h) g(x) = \sum_{q=0}^{p-1} \frac{g^{(q)}(0)}{q!} F(s_h) t^q(x) + \frac{1}{(p-1)} \cdot (F(s_h) t^{p-1} * g^{(p)})(x), \qquad (3.1)$$

and the same holds with s formally in place of s_h . By (1.13),

$$F(s_h) t^{q}(x) - F(s) t^{q}(x) = \frac{1}{2\pi i} \int_{\Gamma} F(\lambda) \cdot \left[(s_h - \lambda)^{-1} t^{q}(x) - (s - \lambda)^{-1} t^{q}(x) \right] \cdot d\lambda.$$

We now substitute $w = \lambda x$ in the integral. Since the contour $x \Gamma$ comes arbitrarily close to the origin for small x, we replace it by an equivalent contour Γ_1 which is independent of $x \in [h, \bar{x}]$, has a positive distance to the origin and, apart from a compact subset, is again contained in a sector $|\arg(-w)| \leq \alpha' < \alpha$.

For $|w| = |\lambda x| \leq \text{const.}$ we obtain from the classical convergence theory of linear multistep methods [3, 9]

$$|(s_h - \lambda)^{-1} t^q(x) - (s - \lambda)^{-1} t^q(x)| \le C \cdot h^{q+1}$$
 for $x \in [h, \bar{x}]$.

For $|\arg(-w)| = |\arg(-\lambda)| \le \alpha' < \alpha$ Lemma 2.1 gives

$$|(s_h-\lambda)^{-1}t^q(x)-(s-\lambda)^{-1}t^q(x)| \leq C \cdot \left(|e^{\lambda x/2}|\cdot h^{q+1}+\frac{\rho^{x/h}}{|\lambda|}\cdot h^q\right).$$

We observe $\rho^{x/h} \leq C \cdot h/x$ and insert the above estimates and the bound in (1.5) into the integral representation over Γ_1 . This yields the estimate

$$|F(s_h) t^q(x) - F(s) t^q(x)| \le C \cdot x^{\mu - 1} \cdot h^{q+1}$$

for $x \in [h, \bar{x}], q = 0, 1, \dots, p-1.$ (3.2)

(The factor $x^{\mu-1}$ comes from $|F(w/x)| \le M \cdot x^{\mu} \cdot |w|^{-\mu}$ and $d\lambda = dw/x$. The integral remains absolutely convergent, because $\mu > 0$.)

Further, for $0 \le x < h$ we have

$$F(s_h) t^{p-1}(x) = \omega_0(h) x^{p-1} = F(\delta_0/h) x^{p-1} = O(h^{\mu+p-1})$$

where we have used (1.5) in the last estimate. Since $f(t) = O(t^{\mu-1})$ as $t \to 0$ we have also

$$F(s) t^{p-1}(x) = O(h^{\mu+p-1})$$
 for $0 \le x < h$.

Using (3.1) we obtain finally the estimate of the theorem. \Box

Convolution Quadrature and Discretized Operational Calculus. I.

We can get rid of the low order error terms in Theorem 3.1 by a simple modification:

$$F(s_h)^{\sim} g(x) = F(s_h) g(x) + \sum_{j=0}^{p-2} w_{nj}(h) g(jh) \quad \text{at} \quad x = nh,$$
(3.3)

where the correction quadrature weights $w_{nj}(h)$ are determined such that the quadrature formula becomes exact for polynomials up to degree p-2:

$$F(s_h)^{\sim} t^q(x) = F(s) t^q(x)$$
 for $q = 0, 1, ..., p-2.$ (3.4)

This gives a Vandermonde system of linear equations for $w_{nj}(h)$. An alternative to (3.4) (for x bounded away from 0) will be given in Corollary 4.2 below.

Corollary 3.2. Under the assumptions (1.5), (1.10) the method (3.3), (3.4) satisfies for $g \in C^{p}[0, \bar{x}]$

$$|F(s_h)^{\sim}g(x) - F(s)g(x)| \leq C \cdot x^{\mu-1} \cdot h^p$$

with C independent of $h \in (0, \overline{h}]$ and $x \in [h, \overline{x}]$.

Proof. With $r(x) = \frac{1}{(p-2)!} (t^{p-2} * g^{(p-1)})(x)$, the remainder in the Taylor expansion of g at 0, we have by (3.4) at x = nh

$$F(s_h)^{\sim} g(x) - F(s) g(x) = F(s_h)^{\sim} r(x) - F(s) r(x)$$

= $F(s_h) r(x) - F(s) r(x) + \sum_{j=0}^{p-2} w_{nj}(h) r(jh).$ (3.5)

The weights $w_{ni}(h)$ are determined from the Vandermonde system

$$\sum_{j=0}^{p-2} w_{nj}(h) \cdot j^q h^q = F(s) t^q(x) - F(s_h) t^q(x) \qquad (q=0, 1, \dots, p-2)$$

where the right-hand side is bounded by $C \cdot x^{\mu-1} \cdot h^{q+1}$ because of Theorem 3.1. Cancelling the factor h^q we see that $w_{ni}(h)$ are bounded by

 $|w_{ni}(h)| \leq C \cdot x^{\mu - 1} \cdot h \qquad (x = nh).$

Moreover,

$$|r(jh)| \leq C \cdot h^{p-1}$$
 for $j = 0, 1, ..., p-2$.

Inserting these estimates in (3.5) and applying Theorem 3.1 (with r instead of g) gives the result. \Box

4. Approximation of the Inverse Laplace Transform

We define $f_n(h)$ by

$$F(\delta(\zeta)/h) = h \sum_{n=0}^{\infty} f_n(h) \zeta^n$$
(4.1)

so that

$$f_n(h) = \omega_n(h)/h \tag{4.2}$$

with $\omega_n(h)$ given by (1.3). We show that $f_n(h)$ approximate the inverse Laplace transform of F(s). For the special case $\delta(\zeta) = 1 - \zeta$ (backward Euler) this is known as the Post-Widder inversion formula [12, 14].

Theorem 4.1. Assume (1.5), (1.10), and let f(t) denote the inverse Laplace transform of F(s). Then

$$|f_n(h) - f(nh)| \leq C \cdot x^{\mu - 1 - p} \cdot h^p \qquad (x = nh)$$

where the constant C does not depend on $h \in (0, \overline{h}]$ and $x \in [h, \overline{x}]$ with fixed $\overline{x} < \infty$.

Remarks. a) For exponentially stable F(s) (i.e., exponentially decaying f) Theorem 4.1 can be extended to a uniform p-th order estimate on the half-line $x \ge 1$, with exponential decay of the (absolute) error.

b) For $F(s) = (s - \lambda)^{-1}$ the coefficients $f_n(h\lambda)$ are the solution of a linear multistep method applied to $y' = \lambda y$ with the special choice of starting values $y_0 = 1/(\delta_0 - h\lambda)$, $y_{-k} = \dots = y_{-1} = 0$. It is rather unexpected that $f_n(h\lambda)$ are *p*-th order approximations to $e^{nh\lambda}$ for *nh* bounded away from 0.

Proof. a) By Cauchy's integral formula,

$$F(\delta(\zeta)/h) = \frac{1}{2\pi i} \int_{\Gamma} \frac{F(\lambda)}{(\delta(\zeta)/h - \lambda)} d\lambda$$

where Γ is again the path of (1.4). We denote the *n*-th coefficient of the power series $(\delta(\zeta) - z)^{-1}$ by $e_n(z)$ and thus have

$$f_n(h) = \frac{1}{2\pi i} \int_{\Gamma} F(\lambda) e_n(h\lambda) d\lambda$$
(4.3)

which closely resembles the inversion formula

$$f(nh) = \frac{1}{2\pi i} \int_{\Gamma} F(\lambda) e^{nh\lambda} d\lambda.$$
(4.4)

We are thus led to study the difference $e_n(h\lambda) - e^{nh\lambda}$. As in the proof of Theorem 3.1, we substitute $w = \lambda x$ (x = nh) and replace the contour $x\Gamma$ by the contour Γ_1 (independent of x) given there.

b) For $z = h\lambda$ with $|\arg(-z)| \leq \alpha' < \alpha$ and $|z| \geq r > 0$ Lemma 2.3a) shows

$$e_n(z) = O\left(\frac{\rho^n}{|z|}\right) = e^{nz} + O\left(\frac{\rho^n}{|z|}\right) \quad \text{for some } \rho < 1.$$
(4.5)

c) Let now $|z| \leq r$, r sufficiently small. As in the proof of Lemma 2.3b) let R(z) be defined by

$$\delta(1/R(z)) = z \tag{4.6}$$

Convolution Quadrature and Discretized Operational Calculus. I.

so that

$$R(z) = e^{z} + O(z^{p+1}).$$
(4.7)

Let first $|\arg(-z)| \leq \alpha' < \frac{\pi}{2}$. Using $|R(z)| \leq |e^{\kappa z}|$ for some $0 < \kappa < 1$, the relation

$$R(z)^{n} - e^{nz} = \sum_{j=0}^{n-1} R(z)^{n-1-j} e^{jz} [R(z) - e^{z}]$$

yields

$$|R(z)^{n} - e^{nz}| \leq C \cdot z^{p} |e^{\kappa nz}| \quad \text{for } |\arg(-z)| \leq \alpha' < \frac{\pi}{2}, |z| \leq r.$$

$$(4.8)$$

Using $|R(z)| \leq e^{\tilde{\kappa}|z|}$ for some $\tilde{\kappa} > 1$, one has the well-known estimate

$$|R(z)^{n} - e^{nz}| \leq C \cdot z^{p} \quad \text{for } |nz| \leq \text{const.}, |z| \leq r.$$
(4.9)

d) We split again

$$\frac{1}{\delta(\zeta) - z} = \frac{1 - R(z)\zeta}{\delta(\zeta) - z} \cdot \frac{1}{1 - R(z)\zeta}$$

and recall that by Cauchy's estimate the coefficients of $(1 - R(z)\zeta)/(\delta(\zeta) - z)$, which we denote by $\gamma_n(z)$, satisfy

$$\gamma_n(z) = O(\rho^n)$$
 for some $\rho < 1$ (uniformly in $|z| \le r$). (4.10)

We write

$$e_n(z) = \sum_{j=0}^n \gamma_j(z) R(z)^{n-j} = R(z)^n \cdot \sum_{j=0}^\infty \gamma_j(z) R(z)^{-j} - \sum_{j=n+1}^\infty \gamma_j(z) R(z)^{n-j}.$$
 (4.11)

The last term is $O(\rho^n)$ for ρ of (4.10), provided that $\rho e^{\kappa r} < 1$ (κ as above). By definition of $\gamma_n(z)$ and by de l'Hospital's rule

$$\sum_{j=0}^{\infty} \gamma_j(z) R(z)^{-j} = \frac{1-R(z)\zeta}{\delta(\zeta)-z} \bigg|_{\zeta=R(z)^{-1}} = \frac{-R(z)}{\delta'(1/R(z))}$$

Differentiating (4.6) we obtain that this expression equals

$$\sum_{j=0}^{\infty} \gamma_j(z) R(z)^{-j} = \frac{R'(z)}{R(z)} = \frac{e^z + O(z^p)}{e^z + O(z^{p+1})} = 1 + O(z^p).$$
(4.12)

Hence we obtain from (4.8) and (4.9)

$$|e_n(z) - e^{nz}| \le C \cdot (z^p |e^{\kappa nz}| + \rho^n)$$
 for $|\arg(-z)| \le \alpha' < \frac{\pi}{2}, |z| \le r,$ (4.13)

$$|e_n(z) - e^{nz}| \leq C \cdot (z^p + \rho^n) \quad \text{for } |nz| \leq \text{const.}, |z| \leq r.$$
(4.14)

e) Inserting the estimates (4.5), (4.13), (4.14) and the bound of (1.5) yields

$$|f_n(h) - f(nh)| = \left| \frac{1}{2\pi i} \int_{\Gamma_1} F\left(\frac{w}{x}\right) \left[e_n\left(\frac{w}{n}\right) - e^w \right] \frac{dw}{x} \right|$$
$$\leq C \cdot x^{\mu - 1} \cdot n^{-p} = C \cdot x^{\mu - 1 - p} \cdot h^p. \quad \Box$$

Theorem 4.1 is also of practical interest in the approximation of F(s) g(x). Let

$$F(s_h)^{\sim} g(x) = F(s_h) g(x) + \sum_{j=0}^{p-2} \omega_{n-j}(h) c_j g(jh) \qquad (x = nh)$$
(4.15)

where c_i do not depend on *n* and *h* (cf. (3.3).)

Corollary 4.2. Assume (1.5), (1.10), and choose c_j in (4.15) as the correction weights of the p-th order Newton-Gregory formula (end-point correction of the trapezoidal rule). Then the method (4.15) satisfies for $g \in C^p[0, \infty)$

$$|F(s_h)^{\sim}g(x) - F(s)g(x)| \leq C \cdot h^p$$

where the constant C does not depend on $h \in (0, \bar{h}]$ and $x = nh \in [x_0, \bar{x}]$ with fixed $x_0 > 0$.

Examples. p=2: $c_0 = -1/2$ (trapezoidal rule) p=3: $c_0 = -7/12$, $c_1 = 1/12$ p=4: $c_0 = -5/8$, $c_1 = 1/6$, $c_2 = -1/24$,

Proof. Let u(t) a smooth function with

$$u(t) = \begin{cases} 0 & \text{for } t \leq x_0/3 \\ 1 & \text{for } t \geq 2x_0/3, \end{cases}$$

and let v(t) = 1 - u(t). By Theorem 3.1,

$$F(s_h)^{\sim}(ug)(x) = F(s)(ug)(x) + O(h^p).$$

Further, at x = nh,

$$F(s_h)^{\sim}(vg)(x) = h \sum_{j=0}^n f_{n-j}(h)(vg)(jh) + h \sum_{j=0}^{p-2} f_{n-j}(h) c_j(vg)(jh)$$

= $h \sum_{j=0}^n f((n-j)h)(vg)(jh) + h \sum_{j=0}^{p-2} f((n-j)h) c_j(vg)(jh) + O(h^p)$
= $F(s)(vg)(x) + O(h^p).$

Here we have used Theorem 4.1 in the second line, and *p*-th order convergence of the Newton-Gregory rule in the last line. Since g = ug + vg, this yields the Newton-Gregory result.

5. Extensions: Derivatives of Convolution Integrals, Non-Smooth Input

In this section we extend Theorem 3.1 in two directions. First we consider the approximation of

$$\left(\frac{d}{dx}\right)^k \int_0^x f(t) g(x-t) dt = s^k F(s) g(x) \qquad (x>0).$$

Theorem 5.1. Under the assumptions (1.5), (1.10) we have for integer $k \ge 0$

$$|s_{h}^{k}F(s_{h})g(x) - s^{k}F(s)g(x)| \leq C \cdot x^{\mu-1-k} \cdot \{h|g(0)| + \dots + h^{p-1}|g^{(p-2)}(0)| + h^{p} \cdot (|g^{(p-1)}(0)| + x|g^{(p)}(0)| + \dots + x^{k}|g^{(p+k-1)}(0)| + x^{k+1}\max_{0 \leq t \leq x}|g^{(p+k)}(t)|)\}$$

where the constant C does not depend on $h \in (0, \bar{h}]$, $x \in [h, \bar{x}]$ with $\bar{x} < \infty$, and $g \in C^{p+k}[0, \bar{x}]$.

Remarks. a) Theorem 5.1 can be interpreted as an extension of Theorem 3.1 to the case $\mu \leq 0$ in (1.5). (Take $\tilde{F}(s) = s^k F(s)$, $\tilde{\mu} = \mu - k$.)

b) For exponentially stable F(s) the result can again be extended to the whole half-line, with exponential decay of the error terms involving $g(0), \ldots, g^{(p+k-1)}(0)$.

- c) Corollary 3.2 remains valid with μk instead of μ .
- d) Theorem 4.1 can be extended similarly.

The proof of Theorem 5.1 is documented in Lubich [11]. For the sake of brevity we shall here only sketch the main arguments.

Outline of the proof. We write

$$s_{h}^{k}F(s_{h})g - s^{k}F(s)g = (s_{h}^{k} - s^{k})F(s)g + s_{h}^{k}(F(s_{h})g - F(s)g).$$

The first term on the right-hand side can be shown to satisfy an estimate of the desired type by using analyticity and growth properties (as $t \rightarrow 0$) of f(t).

The estimate for the second term follows from (1.13) and the error bound

$$|s_{h}^{k}[(s_{h}-\lambda)^{-1}t^{q}-(s-\lambda)^{-1}t^{q}](x)|$$

$$\leq C \cdot \left(|\lambda^{k}e^{\kappa\lambda x}|h^{q+1}+\frac{1}{1+|h\lambda|}\rho^{x/h}\cdot h^{q+1-k}\right) \quad (q=0,1,...,p-1)$$

$$\leq C \cdot \left(|\lambda^{k+p-q-1}e^{\kappa\lambda x}|h^{p}+\frac{1}{1+|h\lambda|}\rho^{x/h}\cdot h^{q+1-k}\right) \quad (q=p,...,p+k-1)$$

where $\kappa > 0$, $\rho < 1$, and C are independent of $h \in (0, 1]$, $x \ge h$ and λ with $|\arg(-\lambda)| \le \alpha' < \alpha$.

This estimate is obtained using techniques similar to those of Sect. 2 and the following asymptotic expansion for R(z) defined in (2.7):

$$R(z)^{n} = e^{nz} \left[1 + P_{1}(nz) z^{p} + \dots + P_{N+1-p}(nz) z^{N} \right] + \operatorname{Rem}(n, z)$$

where P_j are polynomials (of degree *j*), $P_j(0) = 0$, and the remainder satisfies for $|\arg(-z)| \le \alpha' < \frac{\pi}{2}$ and $|z| \le r$ (*r* sufficiently small)

$$|\operatorname{Rem}(n, z)| \leq C |e^{\kappa n z} \cdot z^{N+1}|$$
 for some $\kappa > 0$.

Next we turn to the situation where g(t) is smooth on t > 0, but has an asymptotic expansion in fractional powers of t at t = 0. Here we have the following extension of Theorem 3.1 (or equivalently, of (3.2)). Convergence of order p for $F(s_h)g$ can be restored by eliminating low-order error terms as in Corollary 3.2.

Theorem 5.2. Under the assumptions (1.5), (1.10) we have

$$|F(s_h)t^{\beta-1}(x) - F(s)t^{\beta-1}(x)| \leq \begin{cases} C \cdot x^{\mu-1} \cdot h^{\beta} & \text{for } 0 < \beta \leq p \\ C \cdot x^{\mu-1+\beta-p} \cdot h^{p} & \text{for } \beta \geq p \end{cases}$$
(\$\beta\$ real)

where the constant C is independent of $h \in (0, \bar{h}]$ and $x \in [h, \bar{x}]$ with $\bar{x} < \infty$.

Remark. For $0 < \beta < 1$ the above estimate is understood to hold for

$$F(s_h) g(x) = \sum_{\substack{0 \le jh \le x - h}} \omega_j(h) g(x - jh)$$

which differs from (1.12) in the omission of the last term of the sum, in order that g is not sampled arbitrarily close to the singularity at 0. All the previous results remain valid also for this modified definition.

The proof uses Theorem 5.1 and the following lemma.

Lemma 5.3. Let $\mu, \nu \neq 0, -1, -2, ...$ real numbers. The convolution of two sequences $u_n = O(n^{\mu-1})$ and $v_n = O(n^{\nu-1})$ satisfies

$$\sum_{j=0}^{n} u_j v_{n-j} = O(n^{\gamma-1}), \quad \text{where } \gamma = \max{\{\mu, \nu, \mu+\nu\}}.$$

This result is easily derived using the relation [5, p. 47]

$$(-1)^n \binom{-\mu}{n} = \frac{n^{\mu-1}}{\Gamma(\mu)} [1 + O(n^{-1})].$$

Remark. This formula is the special case $F(s) = s^{-\mu}$, $\delta(\zeta) = 1 - \zeta$, nh = 1 of Theorem 4.1.

Proof of Theorem 5.2. a) If $\beta > p$, we use

$$\frac{t^{\beta-1}}{\Gamma(\beta)} = \frac{t^{p-1}}{\Gamma(p)} * \frac{t^{\beta-p-1}}{\Gamma(\beta-p)}$$

By (2.1) and (2.2),

$$[F(s_h) - F(s)](t^{p-1} * t^{\beta-p-1}) = ([F(s_h) - F(s)]t^{p-1}) * t^{\beta-p-1},$$

and the result follows from (3.2), since $t^{\beta-p-1}$ is locally integrable.

Convolution Quadrature and Discretized Operational Calculus. I.

b) For $\beta < p$ we use

$$\frac{t^{\beta-1}}{\Gamma(\beta)} = s^{p-\beta} \frac{t^{p-1}}{\Gamma(p)}$$

and write

$$[F(s_h) - F(s)] s^{p-\beta} t^{p-1} = [s_h^p(s_h^{-\beta} F(s_h)) - s^p(s^{-\beta} F(s))] t^{p-1} - F(s_h) [s_h^p s_h^{-\beta} - s^p s^{-\beta}] t^{p-1}.$$
(5.1)

By Theorem 5.1 we have for $x \in [h, \bar{x}]$

$$|[s_{h}^{p}(s_{h}^{-\beta}F(s_{h})) - s^{p}(s^{-\beta}F(s))]t^{p-1}(x)| \leq C \cdot x^{\mu+\beta-1-p} \cdot h^{p} \leq C \cdot x^{\mu-1} \cdot h^{\beta}$$
(5.2)

and

$$|[s_{h}^{p}s_{h}^{-\beta} - s^{p}s^{-\beta}]t^{p-1}(x)| \leq C \cdot x^{\beta-1-p} \cdot h^{p}.$$
(5.3)

Further, by (1.5) and Theorem 4.1,

$$|\omega_0(h)| \leq C \cdot h^{\mu}, \quad |\omega_n(h)| \leq C \cdot h^{\mu} \cdot n^{\mu-1} \quad (n \geq 1, nh \leq \bar{x}).$$
(5.4)

By Lemma 5.3 the estimates (5.3), (5.4) yield

$$|F(s_{h})[s_{h}^{p-\beta}-s^{p-\beta}]t^{p-1}(x)| = |\sum_{\substack{0 \leq jh \leq x-h \\ \leq x^{\mu-1} \cdot h^{\beta}}} \omega_{j}(h) \cdot [s_{h}^{p-\beta}-s^{p-\beta}]t^{p-1}(x-jh)|$$
(5.5)

Now (5.1), (5.2) and (5.5) give the result. \Box

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