A new Cubature formula on the Disc for Functions with Singularities, with Error Bound Polyharmonic Paradigm

Ognyan Kounchev

Institute of Mathematics and Informatics, Bulgarian Academy of Sciences, visiting Fraunhofer Institute, Leipzig

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What are Quadrature and Cubature formulas, and what are they good for?

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• Monte Carlo methods - enormous calculations

• Solution of integral equations: we approximate the integral:

$$\int_{a}^{b} K(x, y) f(y) dy = g(x)$$

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$$\int_{a}^{b} K(x, y) f(y) dy \approx \sum_{j=1}^{N} \lambda_{j} K(x, y_{j}) f(y_{j})$$

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- Application to Interpolation theory

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One-dimensional reminder on quadrature formulas

• The *N*-point Quadrature formula of Gauss:

$$\int_{-1}^{1} t^{k} dt \approx \sum_{j=1}^{N} \lambda_{j} t_{j}^{k} = G_{N} \left[t^{k} \right] \quad \text{for } k = 0, 1, ..., 2N - 1$$
$$-1 < t_{j} < 1, \ \lambda_{j} > 0,$$

i.e. exact for polynomials f with deg $f \leq 2N - 1$;

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• **THEOREM**. If $P_N(t)$ is the orthogonal polynomial of degree N i.e.

$$\int_{-1}^{1}t^{j}P_{N}\left(t
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 for $j=0,1,...,N-1$

then

$$P_{N}(t_{j}) = 0$$
 for $j = 1, 2, ..., N$

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• For the polynomials $P_N(t) - 3$ -term recurrence relations which reduces the computation of the knots t_j to a simple and fast Linear Algebra.

• What if f(t) is singular at t = -1 or at t = 1???

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- For a continuous weight function w(t) > 0 (originally, Jacobi's weight $w(t) = (1+t)^{\alpha} (1-t)^{\beta}$) let

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- We have N-point Gauss-Jacobi formula

$$\int_{-1}^{1} t^{k} w(t) dt \approx \sum_{j=1}^{N} \lambda_{j} t_{j}^{k} w(t_{j}) =: GJ_{N} \left[t^{k} \right] \quad \text{for } k = 0, 1, ..., 2N - 1$$

where $P_{N}(t_{j}) = 0$ and $\lambda_{j} > 0$, but
 $\int_{-1}^{1} t^{j} P_{N}(t) w(t) dt = 0 \quad \text{for } j = 0, 1, ..., N - 1.$

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• Example: Compute

$$\int_{0}^{1} g\left(t\right) \frac{1}{\sqrt{t}} dt$$

in two ways: using **Gauss** G_N , or Gauss-Jacobi G_M , for $w(t) = \frac{1}{\sqrt{t}} \log C$

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Important for us is the following remarkable inequality:

ullet Consider all measures $d\mu \geq 0$ (Stieltjes measures) such that

$$\int_{-1}^{1} t^{k} d\mu(t) = \sum_{j=1}^{N} \lambda_{j} t_{j}^{k} = G J_{N} \left[t^{k} \right] \quad \text{for } k = 0, 1, ..., 2N - 1$$

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• Then

$$\int_{-1}^{1} t^{2N} d\mu\left(t\right) \geq \sum_{j=1}^{N} \lambda_{j} t_{j}^{2N} = G J_{N}\left[t^{2N}\right]$$

Gauss (30.04.1777 in Brauhschweig - 23.02.1855)

Wiki: "His mother was illiterate and never recorded the date of his birth, remembering only that he had been born on a Wednesday... Gauss was a child prodigy. "



Carl Gustav Jacobi (10.12.1804 in Potsdam - 18.02.1851)

Jacobi was a prodigy as well. Wiki: "However, as the University was not accepting students younger than 16 years old, he had to remain in the senior class until 1821."



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Important: there is Error bound for Gauss-Jacobi quadratures

In the case of smooth functions f ∈ C^{2N} (a, b) holds the A. A.
 Markov estimate:

$$\left|\int_{-1}^{1} f(t) w(t) dt - \sum_{j=1}^{N} \lambda_{j} f(t_{j})\right| \leq \frac{\left\|f^{(2N)}\right\|}{(2N)!\kappa_{N}^{2}}$$

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 Here κ_N is the leading coefficient of the orthonormal polynomial P_N w.r.t. the weight w (t) dt.

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Andrei Andreevich Markov (14.06.1856 in Ryazan - 20.07.1922)

Wiki: "He attended Petersburg Grammar, he was seen as a **rebellious student** by a select few teachers. In his academics he **performed poorly** in most subjects other than mathematics (which later became his profession)."

"He figured out that he could use chains to model the alliteration of vowels and consonants in Russian literature"



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Pafnutii Lvovich Chebyshev (May 16, 1821 - 1894)

Wiki: "Chebyshev mentioned that his music teacher also played an important role in his education, for she "raised his mind to exactness and analysis"... His disability prevented his playing many children's games and he devoted himself instead to mathematics"



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• The usual Cubature formulas: Solve for λ_j and x_j the equations

$$\int_{D} x^{m} dx = \sum_{j=1}^{N} \lambda_{j} \left[x^{(j)} \right]^{m} \quad \text{for } m = (m_{1}, m_{2}, ..., m_{n}) \in M \subset \mathbb{Z}^{n}$$
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• Example: Padua points.

Example of tensor Cubature formulas and its error bounds

• Tensor product Cubature formulas on tensor product domains (rectangle):

$$I[f] := \int_0^1 \int_0^1 f(x, y) \, dx \, dy = \int_0^1 I_1(x) \, dx$$
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• The tensor product **Trapezoidal rule** $T_N[f]$ with step $h = \frac{1}{N}$, uses the values

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$$f\left(\frac{j_1}{N},\frac{j_2}{N}\right)$$
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• The error bound is:

$$\operatorname{Error} = |I[f] - T_N[f]| \le \frac{A_1 + A_2}{12N^2}$$
$$A_1 = \max_{0 \le x, y \le 1} \left| \frac{\partial^2 f}{\partial x^2} \right|, \quad A_2 = \max_{0 \le x, y \le 1} \left| \frac{\partial^2 f}{\partial y^2} \right|$$

Cubature formulas in the disc

• Consider Cubature formulas on the **unit disc** $B \subset \mathbb{R}^2$:

$$\int_{B} f(x) dx \approx \sum_{j=1}^{N} \lambda_{j} f\left(x^{(j)}\right) =: C_{N}[f].$$

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• E.g.

$$w(x_1, x_2) = \frac{1 + x_1}{\|x\|}$$
 or $w(x_1, x_2) = |x_1|$.

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• Explain only 2D case: Expand in Fourier series P and w, with $z = x + iy = re^{i\varphi}$:

$$P(z) = \sum_{k=-\infty}^{\infty} p_k(r) e^{ik\varphi} \qquad w(z) = \sum_{k=-\infty}^{\infty} w_k(r) e^{ik\varphi}$$

where

$$p_{k}(r) := \frac{1}{2\pi} \int_{0}^{2\pi} P\left(re^{i\varphi}\right) e^{-ik\varphi} d\varphi; \quad w_{k}(r) := \frac{1}{2\pi} \int_{0}^{2\pi} w\left(re^{i\varphi}\right) e^{-ik\varphi} d\varphi;$$

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Our approach

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where

$$p_{k}\left(r\right):=\frac{1}{2\pi}\int_{0}^{2\pi}P\left(re^{i\varphi}\right)e^{-ik\varphi}d\varphi;\quad w_{k}\left(r\right):=\frac{1}{2\pi}\int_{0}^{2\pi}w\left(re^{i\varphi}\right)e^{-ik\varphi}d\varphi;$$

Hence,

$$I = \int_{B} P(z) w(z) dz = 2\pi \sum_{k=-\infty}^{\infty} \int_{0}^{1} p_{k}(r) w_{-k}(r) r dr$$

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• Gauss-Almansi representation ($z = r \times e^{i\varphi}$, r = |z|):

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- This is related to the so-called **Polyharmonic Paradigm.**
- See more about it in the monograph "Multivariate Polysplines. Applications to Numerical and Wavelet Analysis", Academic Press, 2001.

The integral as infinite sum of 1-dim integrals

Hence, for polynomials $P\left(x
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$$I = \sum_{k} \int_{0}^{1} P_{k}(r^{2}) r^{k} w_{k}(r) r dr = \sum_{k} \int_{0}^{1} P_{k}(\rho) \widetilde{w}_{k}(\rho) d\rho;$$

• Here the new weigth $\widetilde{w}_{k,\ell}(\rho)$ is defined by

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 OUR MAIN CONSTRUCTION: For every k ∈ Z and N ≥ 1, apply N-point Gauss-Jacobi quadrature:

$$\int_{0}^{1} P_{k}\left(\rho\right) \widetilde{w}_{k}\left(\rho\right) d\rho \approx \sum_{j=1}^{N} P_{k}\left(t_{j;k}\right) \lambda_{j;k}$$

It is exact for polynomials P_k satisfying deg $P_k \leq 2N - 1$.

The cubature formula defined:

Let g(x) be **arbitrary continuous** function with Fourier expansion

$$g\left(x
ight)=\sum_{k=-\infty}^{\infty}g_{k}\left(r
ight)e^{ikarphi}$$

The integral becomes

$$I[g] = \int_{B} g(z) w(z) dz = \sum_{k} \int_{0}^{1} g_{k}(r) w_{k}(r) r dr$$
$$= \frac{1}{2} \sum_{k} \int_{0}^{1} g_{k}(\sqrt{\rho}) \rho^{-\frac{k}{2}} \rho^{\frac{k}{2}} w_{k}(\sqrt{\rho}) d\rho$$
$$\approx \frac{1}{2} \sum_{k=-\infty}^{\infty} \sum_{j=1}^{N} g_{k}(\sqrt{t_{j;k}}) t_{j;k}^{-\frac{k}{2}} \times \lambda_{j;k}$$
$$=: C(g)$$

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• Convergence of *C*(*g*):

$$2C(g) = \sum_{k} \sum_{j=1}^{N} g_k \left(\sqrt{t_{j;k}} \right) \cdot t_{j;k}^{-\frac{k}{2}} \cdot \lambda_{j;k} < \infty.$$

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- We obtain

$$\left|\sum_{j=1}^{N} g_{k}\left(t_{j;k}\right) \cdot t_{j;k}^{-\frac{k}{2}} \cdot \lambda_{j;k}\right| \leq C \left\|g\right\|_{\sup} \int w_{k}\left(\sqrt{\rho}\right) d\rho$$

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- The proof: application of the famous Chebyshev inequality.
- We obtain

$$\left|\sum_{j=1}^{N} g_{k}\left(t_{j;k}\right) \cdot t_{j;k}^{-\frac{k}{2}} \cdot \lambda_{j;k}\right| \leq C \left\|g\right\|_{\sup} \int w_{k}\left(\sqrt{\rho}\right) d\rho$$

• Further, we impose the condition

$$\|w\| := \sum_{k} \int |w_{k}(\sqrt{\rho})| \, d\rho < \infty$$

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To finish the Cubature formula, approximate the coefficients $g_k(r)$. In \mathbb{R}^2 we have

$$egin{aligned} \mathsf{g}_{k}\left(r
ight) =rac{1}{2\pi}\int_{0}^{2\pi}\mathsf{g}\left(r\mathsf{e}^{iarphi}
ight) \mathsf{e}^{ikarphi}\mathsf{d}arphi \end{aligned}$$

Hence, for integers $M \ge 1$, use the **trapezoidal rule**:

$$f_{k}^{\left(M\right)}\left(r\right) := \frac{2\pi}{M} \sum_{s=1}^{M} f\left(r e^{j\frac{2\pi s}{M}}\right) e^{j\frac{2\pi s}{M}}$$

The final Cubature formula is:

$$\int_{B} g(z) w(z) dz \approx \frac{\pi}{M} \sum_{k=0}^{K} \sum_{j=1}^{N} \sum_{s=1}^{M} \lambda_{j,k} \cdot t_{j,k}^{-\frac{k}{2}} \cdot e^{i\frac{2\pi s}{M}} \cdot g\left(\sqrt{t_{j,k}} e^{i\frac{2\pi s}{M}}\right)$$

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• The nodes are

$$\sqrt{t_{j,k}}e^{jrac{2\pi s}{M}}$$
 $0 \leq s \leq M-1, \ |k| \leq K, \ j=1,...,N$

and the weights are

$$\lambda_{j,k} \cdot t_{j,k}^{-\frac{k}{2}} \cdot e^{i\frac{2\pi s}{M}}$$

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• The formula is exact for the polynomials

$$P(x,y) = r^{2s}r^k e^{ik\varphi} = |z|^{2s}z^k$$

for $0 \le s \le 2N - 1$; $0 \le k \le M - 1 - K$

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• The coefficients satisfy the stability estimate

$$\frac{\pi}{M}\sum_{k=0}^{K}\sum_{j=1}^{N}\sum_{s=1}^{M}\left|\lambda_{j,k}\cdot t_{j,k}^{-\frac{k}{2}}\cdot e^{j\frac{2\pi s}{M}}\right|\leq C_{1}\|w\|.$$

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• By a theorem of Polya and others, we have a stable Cubature formula.

• **nice Error estimates** for these Cubature formula, w.r.t. all parameters *K*, *N*, *M*.

Details will appear in a book:

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- **nice Error estimates** for these Cubature formula, w.r.t. all parameters *K*, *N*, *M*.
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• O. Kounchev, H. Render, The Multidimensional Moment problem, Hardy spaces, and Cubature formulas, in preparation for Springer • For

$$w = \frac{1+x}{\sqrt{x^2+y^2}} = \frac{1}{r} + \cos\varphi$$

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• For functions

$$\begin{split} f_0\left(x,y\right) &= 1 + x^4 + y^3, \\ f_1\left(x,y\right) &= 1 + \frac{x^3}{\sqrt{x^2 + y^2}} + \frac{y^7}{x^2 + y^2} = 1 + r^2\cos^3\varphi + r^5\sin^7\varphi, \\ f_2\left(x,y\right) &= \cos\left(10x + 20y\right), \\ f_3\left(x,y\right) &= \left(x^2 + y^2\right)^{5/4} = r^{5/2} \end{split}$$

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TABLE 1

N/M	9	25	63	83
10	0.00000903315016	0.00000903315016	0.00000903315016	0.00
15	0.00000195087406	0.00000195087406	0.00000195087406	0.00
25	0.00000027232575	0.00000027232575	0.00000027232575	0.00
35	0.0000007324233	0.0000007324233	0.0000007324233	0.00
50	0.0000001802778	0.00000001802778	0.00000001802778	0.00

Error of
$$C_{N,M}^1$$
 for $f_1 w^{(1)} = \left(1 + r^2 \cos^3 \varphi + r^5 \sin^7 \varphi\right) \left(rac{1}{r} + \cos \varphi\right)$

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TABLE 2

N\M	9	25	63	83
10	0.38233156987266	0.01278813623111	0.0000006432655	0.00
15	0.38233496964021	0.01278820055772	0.0000000000000000	0.00
25	0.38233500750838	0.01278820055772	0.0000000000000000	0.00
35	0.38233500770641	0.01278820055772	0.0000000000000000	0.00
50	0.38233500771330	0.01278820055772	0.0000000000000000	0.00

Error of
$$C_{N,M}^1$$
 for $f_2 w^{(1)} = (\cos(10x + 20y))\left(\frac{1}{r} + \cos\varphi\right)$

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 ${\rm TABLE}\ 3$

N/M	9	25	63	8
10	0.000062570230356	0.000062570230356	0.000062570230356	C
15	0.000015507227945	0.000015507227945	0.000015507227945	C
25	0.000002648868861	0.000002648868861	0.000002648868861	C
35	0.000000823451885	0.000000823451885	0.000000823451885	C
50	0.000000237995663	0.000000237995663	0.000000237995663	C

Error of
$$C_{N,M}^1$$
 for $f_3 w^{(1)} = r^{5/2} \left(\frac{1}{r} + \cos \varphi \right)$

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We compare with the *piecewise midpoint quadrature rule*. It is rather geometric: subdivide the disk of radius R by concentric circles of radius

$$r_{j} = rac{j^{2} - j + 1/3}{j - rac{1}{2}} rac{R}{N} \; pprox rac{j}{N} R$$
 for $j = 1, ..., N$

and radial half-lines with angle $2\pi i/M$ for i = 1, ..., M. The *piecewise midpoint quadrature rule*, is given by:

$$I_{N,M}^{\text{mid}}(f) := \frac{2\pi R^2}{M \cdot N^2} \sum_{j=1}^{N} \sum_{s=1}^{M} \left(j - \frac{1}{2} \right) f\left(r_j \cos \frac{2\pi \left(s - \frac{1}{2} \right)}{M}, r_j \sin \frac{2\pi \left(s - \frac{1}{2} \right)}{M} \right)$$

TABLE 4

N=M	$I_{N,N}^{\text{mid}}\left(f_{0}w^{(1)}\right)$	Error
5	6. 293 948 149 525 97	0.460 476 055 692 09
10	6. 552 664 285 742 99	0.201 759 919 475 07
20	6. 652 725 619 004 72	0.101 698 586 213 34
100	6. 733 953 574 717 90	0.020 470 630 500 16
200	6. 744 180 708 690 65	0.010 243 496 527 41

Midpoint cubature for $f_0 w^{(1)} = (1 + x^4 + y^3) \left(\frac{1}{r} + \cos \varphi\right)$

True Value is: $\frac{43}{20}\pi \approx 6.754\,424\,205\,218\,060$

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TABLE 5

N=M	$I_{N,N}^{\text{mid}}\left(f_{1}w^{(1)}\right)$	Error
5	6.479 185 720 369 13	0.393048209358541
10	6.671 455 800 859 80	0.200778128867871
20	6.770 780 856 013 81	0.101453073713858
100	6.851 773 117 091 46	0.020460812636194
200	6.861 992 887 600 82	0.010241042126847

Midpoint cubature for
$$f_1 w^{(1)} = \left(1 + r^2 \cos^3 \varphi + r^5 \sin^7 \varphi\right) \left(\frac{1}{r} + \cos \varphi\right)$$

True value is $\approx 6.872\,233\,929\,727\,67$

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• For given N, let ρ_j , j = 1, ..., N be the nodes of the Gauss quadrature G_N on $[0, R^2]$ with corresponding weights w_j , further α be a real parameter and M a natural number: then the **generalized Peirce cubature** is:

$$I_{N,M}^{\mathsf{Peirce},\alpha}\left(f\right) := \frac{\pi}{M} \sum_{j=1}^{N} w_j \sum_{s=1}^{M} f\left(\sqrt{\rho_j} \cos \frac{2\pi \left(s+\alpha\right)}{M}, \sqrt{\rho_j} \sin \frac{2\pi \left(s+\alpha\right)}{M}\right)$$

is called .

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is called .

• The usual cubature of Peirce is obtained by setting N = m + 1, M = 4m + 4, and $\alpha = 0$.

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The hybrid cubature by spline interpolation

 A drawback of our formula: High number of evaluations points is needed in our formula – we need (2K − 1) · N · M evaluation points.

The hybrid cubature by spline interpolation

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- We solve the problem by using spline interpolation: We use point evaluations on a regular grid in both directions φ and r, where the number of knots is $N_1 \times M$, and N_1 is the number of spline knots in direction r.

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- We solve the problem by using spline interpolation: We use point evaluations on a regular grid in both directions φ and r, where the number of knots is $N_1 \times M$, and N_1 is the number of spline knots in direction r.
- The **hybrid cubature** uses splines methods with a cubature formula. It has the form:

$$C_{N,M}^{K}(f) \approx \frac{1}{2} \sum_{k=0}^{K} \sum_{\ell=1}^{a_{k}} \sum_{j=1}^{N} SPL\left[\{R_{m}\}_{m=0}^{N_{1}}; \{f_{(k,\ell)}^{(M)}(R_{m})\}_{m=0}^{N_{1}} \right] \left(\sqrt{t_{j,(k,\ell)}} \right]$$

where $SPL\left[\{R_m\}_{m=0}^{N_1}; \{V_m\}_{m=0}^{N_1}\right](t)$ is the value at t of a univariate spline interpolation function with nodes $\{R_m\}_{m=0}^{N_1}$ for the data $\{V_m\}_{m=0}^{N_1}$.

Details are available in the following references:

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