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OPTIMAL KNOTS FOR K - FOLD LAGRANGIAN NUMERICAL DIFFERENTIATION

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<u>1. Introduction.</u> Let L_n be the Lagrangian interpolation polynomial for $f: I \to \mathbb{R}$, $I = [-1,1]$, and $N := n + 1$ knots $-1 \le x_o < x_1 < \dots < x_n \le 1$. For $f \in C^k(I)$, $k \in \mathbb{N}$, the approximation of $f^{(k)}$ by $L_n^{(k)}$ is denoted as <u>k-fold Lagrangian numerical differentiation.</u> For $f \in C^N(I)$ the (truncation-) error can be represented as

$$(1) \quad R_N(f,x,k) := f^{(k)}(x) - L_n^{(k)}(x) = \frac{1}{N!} H^{(k)}(x) f^{(N)}(\xi_k(x)) , \quad \xi_k(x) \in I,$$

$k = 1,2,\dots, N-2$, exactly in all points $x \in I$ satisfying the condition

$$(2) \quad g(x) := \left[H^{(k)}(x) - k \left(\frac{H(x)}{x-x_o} \right)^{(k-1)} \right] \cdot \left[H^{(k)}(x) - k \left(\frac{H(x)}{x-x_n} \right)^{(k-1)} \right] \ge o ,$$

where $H(x) := (x-x_o)(x-x_1)\dots(x-x_n)$ (cf. [5] for $k = 1$, [4] for $k \ge 2$).

<u>2. The set D_k.</u> For fixed k let $D_k := \{x \in I \,/\, g(x) \ge o\}$. In order to determine the set D_k practically it is necessary to obtain a general view of the zeros of the polynomial $g \in \Pi_{2(n+1-k)}$. Obviously g can be brought to the form

$$(3) \quad g(x) = (x-x_o) \cdot \left[\frac{H(x)}{x-x_o} \right]^{(k)} \cdot (x-x_n) \cdot \left[\frac{H(x)}{x-x_n} \right]^{(k)} .$$

Thus $g(x_o) = g(x_n) = o$ and $g(x) > o$ for $x < x_o$ and $x > x_n$.

<u>Theorem 1.</u> g has $2(n-k)$ simple and distinct zeros in (x_o,x_n), and the measure of the set D_k is

$$|D_k| = 2 - \frac{k}{n}(x_n - x_o) .$$

Proof. The following lemma of V.A. Markov [2] will be applied: Let

$$p(x) := (x-c_1)\dots(x-c_s)\ ,\ q(x) := (x-b_1)\dots(x-b_s)$$

where

$$b_1 > \dots > b_s,\ c_1 > \dots > c_s\ ,\ b_1 \geq c_1 \geq \dots \geq b_s \geq c_s$$

and $b_j \neq c_j$ for at least one index j. Then for $1 \leq k \leq s-1$ the zeros $\gamma_1 > \dots > \gamma_{s-k}$ resp. $\beta_1 > \dots > \beta_{s-k}$ of $p^{(k)}$ resp. $q^{(k)}$ are satisfying the inequality $\beta_1 > \gamma_1 > \dots > \beta_{s-k} > \gamma_{s-k}$.

In this case let

$$p(x) := \frac{H(x)}{x-x_n} = (x-x_{n-1})\dots(x-x_o),$$

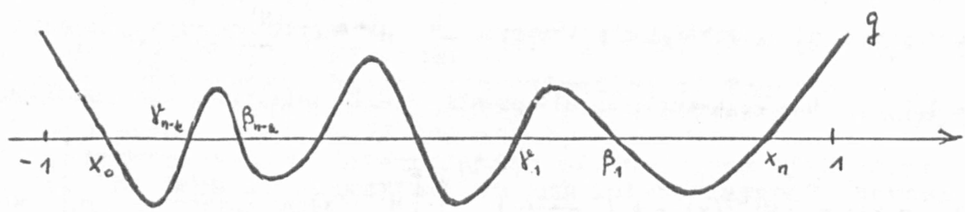
$$q(x) := \frac{H(x)}{x-x_o} = (x-x_n)\dots(x-x_1)$$

and $c_i := x_{n-i},\ b_i := x_{n+1-i}\ ,\ i=1,\ \dots,\ n$.

Case 1 : $1 \leq k \leq n-1$.

Markov's lemma gives for the zeros $\gamma_1 > \dots > \gamma_{n-k}$ resp. $\beta_1 > \dots > \beta_{n-k}$ of $p^{(k)}$ resp. $q^{(k)}$ the inequality $\beta_1 > \gamma_1 > \dots > \beta_{n-k} > \gamma_{n-k}$.

Thus the graph of g can be represented as follows



and consequently

$$|D_k| = (1-x_n) + (x_o+1) + \sum_{i=1}^{n-k} (\beta_i - \gamma_i)\ .$$

In order to calculate the sum on the right hand side it has to be observed that

$$p(x) = x^n - (\sum_{i=o}^{n-1} x_i)\, x^{n-1} + \tilde{p}(x)\ ,\quad \tilde{p} \in \Pi_{n-2}\ .$$

k-fold differentiation gives

$$p^{(k)}(x) = \frac{n!}{(n-k)!} x^{n-k} - \frac{(n-1)!}{(n-1-k)!} (\sum_{i=o}^{n-1} x_i)\, x^{n-1-k} + \tilde{p}^{(k)}(x).$$

Since on the other side $\gamma_1, \dots, \gamma_{n-k}$ are the zeros of $p^{(k)}$, we obtain

$$p^{(k)}(x) = \frac{n!}{(n-k)!}(x-\gamma_1)\dots(x-\gamma_{n-k})$$

$$= \frac{n!}{(n-k)!}x^{n-k} - \frac{n!}{(n-k)!}\left(\sum_{i=1}^{n-k}\gamma_i\right)x^{n-1-k} + \tilde{p}^{(k)}(x) .$$

Comparing the coefficients of x^{n-k-1} yields

$$\sum_{i=1}^{n-k}\gamma_i = \frac{n-k}{n}\sum_{i=0}^{n-1}x_i$$

and in a similar way for $q^{(k)}$

$$\sum_{i=1}^{n-k}\beta_i = \frac{n-k}{n}\sum_{i=1}^{n}x_i .$$

With these results we obtain as stated

$$|D_k| = (1-x_n) + (x_o+1) + \frac{n-k}{n}\left(\sum_{i=1}^{n}x_i - \sum_{i=o}^{n-1}x_i\right) = 2 - \frac{k}{n}(x_n - x_o).$$

Case 2 : $k = n$.

$p^{(n)}(x) = q^{(n)}(x) = n!$ gives $g(x) = (x-x_o)(x-x_n)(n!)^2$

and consequently $|D_n| = (1-x_n) + (x_o+1) = 2-(x_n-x_o)$.

This completes the proof of the theorem.

Roughly speaking Theorem 1 says that (1) holds at "almost all" points $x \in I$ for N large enough.

3. Optimization. In the following section the task will be to minimize $|R_N(f,x,k)|$ on D_k in a proper sense by choosing suitable distinct and simple knots $x_i \in I$. Since $f^{(N)}$ is assumed to be uniformly bounded on I, the order of the right hand side in (1) is determined by $H^{(k)}$. Therefore it is reasonable to measure the error either by the sup - norm $\|\cdot\|_\infty$ (cf. Salzer [3]) or by a weighted euclidean norm $\|\cdot\|_{2,w}$ (cf. Schönhage [5] for $k = 1$) and to call the knots optimal iff $\|H^{(K)}\|_\infty$ resp. $\|H^{(k)}\|_{2,w}$ (in both cases with respect to I) attains its minimum. In the present paper the second measure will be considered especially for $k \geq 2$.

4. Optimal knots for $w(x)=(1-x)^\alpha(1+x)^\beta$, $\alpha,\beta > -1$. We must attempt to minimize

(4) $$\|H^{(k)}\|_{2,w} = \left[\int_{-1}^{1}(1-x)^\alpha(1+x)^\beta[H^{(k)}(x)]^2dx\right]^{1/2} \quad \text{for } \alpha, \beta > -1.$$

It is well known that for any weightfunction w there exists an orthonormal system of polynomials $g_o, g_1, \ldots, g_n \in \Pi_n$, on I. If $H^{(k)} \in \Pi_{N-k}$ is developed with respect to these polynomials,

$$H^{(k)}(x) = \sum_{i=o}^{N-k} a_i\, g_i(x) \;,$$

then a_{N-k} is determined by the leading coefficient $\frac{N!}{(N-k)!}$ of $H^{(k)}$ and in this way independant of the knots x_i and different from zero. Since

$$\| H^{(k)} \|_{2,w} = \left[\sum_{i=o}^{N-k} a_i^2 \right]^{1/2} \;,$$

the minimum in (4) is attained iff

(5) $$H^{(k)}(x) = c\, g_{N-k}(x),\; c \in \mathbb{R} \;,$$

i.e. the optimal knots have to be chosen as the zeros of a k-fold primitive of the polynomial g_{N-k}. In determining this k-fold primitive it is necessary to add an arbitrary polynomial of degree $k-1$. Therefore the question arises if there exists a k-fold primitive of g_{N-k} possessing N simple and distinct zeros in I.

The system of orthonormal polynomials on I belonging especially to the above mentioned weight function $w(x) = (1-x)^{\alpha}(1+x)^{\beta}$, $\alpha,\beta > -1$, is the system of Jacobi-polynomials $P_N^{(\alpha,\beta)}$, $N \in \mathbb{N}_o$, with the normalizing integral

(6) $$\int_{-1}^{1} (1-x)^{\alpha}(1+x)^{\beta} \,[\, P_N^{(\alpha,\beta)}(x)]^2 dx = \frac{2^{\alpha+\beta+1}\, \Gamma(N+\alpha+1)\,\Gamma(N+\beta+1)}{(2N+1+\alpha+\beta)\; N!\; \Gamma(N+\alpha+\beta+1)} \,.$$

The Rodrigues - formula [6] yields for arbitrary real parameters α,β the generalized Jacobi - polynomials

$$P_N^{(\alpha,\beta)}(x) = \sum_{i=o}^{N} \binom{N+\alpha}{N-i} \binom{N+\beta}{i} \left(\frac{x-1}{2}\right)^{i} \left(\frac{x+1}{2}\right)^{N-i} ,\; x \in \mathbb{R}$$

of degree $N \in \mathbb{N}_o$ with the properties

(7) $$P_N^{(\alpha,\beta)}(1) = \binom{N+\alpha}{N} ,\quad P_N^{(\alpha,\beta)}(-1 = (-1)^N \binom{N+\beta}{N} ,$$

(8) $$[P_N^{(\alpha-1,\beta-1)}(x)]' = \frac{1}{2}\,(N+\alpha,\beta-1) P_{N-1}^{(\alpha,\beta)}(x) \;,\quad N \in \mathbb{N} ,$$

$$(9)\qquad (1-x)^{\alpha-1}(1+x)^{\beta-1}\, P_N^{(\alpha-1,\beta-1)}(x) = -\frac{1}{2N}\left[(1-x)^{\alpha}(1+x)^{\beta}\, P_{N-1}^{(\alpha,\beta)}(x)\right]', \quad N \in \mathbb{N}.$$

Essentially equation (8) says that differentiation resp. integration of a generalized Jacobi-polynomial can be achieved by shifting the parameters α and β. Induction on k gives easily

$$(10)\qquad \left[P_N^{(\alpha-k,\beta-k)}(x)\right]^{(k)} = P_{N-k}^{(\alpha,\beta)}(x)\,\frac{1}{2^k}\prod_{i=o}^{k-1}(N+\alpha+\beta-k-i)\,,\quad N \geq k.$$

Comparing (10) and (5) suggests to put

$$g_{N-k} = P_{N-k}^{(\alpha,\beta)}.$$

A special k-fold primitive of g_{N-k} is the generalized Jacobi-polynomial $P_N^{(\alpha-k,\beta-k)}$ (apart from a constant), and it remains to show that this polynomial has indeed N simple and distinct zeros in I (under suitable restrictions on the parameters).

Theorem 2. For $\alpha, \beta > k-2$, $N \geq \max[k, 2k-1-(\alpha+\beta)]$, the generalized Jacobi-polynomial $P_N^{(\alpha-k,\beta-k)}$ has N simple and distinct zeros $x_o < x_1 < \ldots < x_{N-1}$, where

$$x_{N-1} = 1 \quad \text{for} \quad \alpha = k-1\,,$$

$$1 < x_{N-1} \leq + \frac{2|\alpha-k+1|}{N(N+\alpha+\beta-2k+1)} \qquad \text{for} \quad k-2 < \alpha < k-1\,,$$

$$x_o = -1 \quad \text{for} \quad \beta = k-1\,,$$

$$-1-\frac{2|\beta-k+1|}{N(N+\alpha+\beta-2k+1)} \leq x_o < -1 \quad \text{for} \quad k-2 < \beta < k-1\,,$$

$$-1 < x_i < 1\,,\ i = o, \ldots, N-1, \text{ otherwise.}$$

Following the lines of Schönhage's proof for $k = 1$ [5, pp. 31o – 311] the proof of theorem 2 can be given by induction on k, using (7), (8), (9) and discussing seven different cases in each step of the proof.

Corollary. Exactly for $\alpha, \beta \geq k-1$ $P_N^{(\alpha-k,\beta-k)}$ has N simple and distinct zeros in I, being optimal knots for the k-fold Lagrangian numerical differentiation in the sense of (4).

5. The special case $\alpha = \beta = k - 1$. In this case the Jacobi - polynomial $P_N^{(\alpha-k,\beta-k)}$ is for any k reduced to $P_N^{(-1,-1)}$, being on account of (8) representable as an integrated Legendre - polynomial,

$$P_N^{(-1,-1)}(x) = \frac{N-1}{2} \int_{-1}^{x} P_{N-1}(t)dt \quad ,$$

and having according to theorem 2 all its zeros in I. The leading coefficient is

$$a_N = \frac{1}{2^N} \binom{2N-2}{N} \quad . \tag{11}$$

Putting

$$H(x) = \frac{1}{a_N} P_N^{(-1,-1)}(x)$$

yields after some elementary calculations utilizing (10) and (6)

$$\| H^{(k)} \|_{2,w} = \frac{N-1}{a_N} \sqrt{\frac{(N+k-2)!}{2(2N-1)(N-k)!}} \;, \quad N \geq k+1 \;, \tag{12}$$

where $w(x) = (1-x)^{k-1}(1+x)^{k-1}$, and by (1) the error estimation

$$|R_N(f,x,k)| \leq c(N,k) \| f^{(N)} \|_{2,w} \;, \quad N \geq k+1 \;, \quad x \in D_k \;, \tag{13}$$

can be obtained where

$$c(N,k) = \frac{N-1}{a_N N!} \sqrt{\frac{(N+k-2)!}{2(2N-1)(N-k)!}} \quad .$$

For $k = 2$ some numerical values of these factors are:

N	c(N,2)
6	$0.13\ 48\ 11\ 29 \cdot 10^{-4}$
7	$0.95\ 72\ 46\ 75 \cdot 10^{-6}$
8	$0.59\ 52\ 48\ 13 \cdot 10^{7}$
9	$0.32\ 90\ 89\ 65 \cdot 10^{-8}$

Making use of the fact that

$$\| f^{(N)} \|_{2,w} = [\int_{-1}^{1} (1-x)^{k-1}(1+x)^{k-1}[f^{(N)}(x)]^2 dx]^{1/2}$$

$$\leq \| f^{(N)} \|_\infty \; [\int_{-1}^{1} (1-x^2)^{k-1} dx]^{1/2} = \sqrt{r(k)} \; \| f^{(N)} \|_\infty \; ,$$

where $$r(k) = 2 \sum_{i=o}^{k-1} \binom{k-1}{i} \frac{(-1)^i}{2i+1} \; ,$$

k	1	2	3	4	5	6	7	8
r(k)	2	$\frac{4}{3}$	$\frac{16}{15}$	$\frac{32}{25}$	$\frac{256}{315}$	$\frac{512}{693}$	$\frac{2048}{3003}$	$\frac{4096}{6435}$

the error estimation (13) can be brought to the form

(14) $$|R_N(f,x,k)| \sqrt{r(k)} \; C(N,k) \; \| f^{(N)} \|_\infty \; , \quad N \geq k+1 \; , \quad x \in D_k \; .$$

It should be observed that by the choice of the parameters α and β as above the same set of knots is optimal for arbitrary k-th derivatives, of course with respect to the weightfunction $w(x) = (1-x)^{k-1}(1+x)^{k-1}$ depending on k.

6. Final remarks. Numerical experiments have certified the remarkable accuracy of this method also on $I \setminus D_k$. The following table (cf. [1]) shows for $k = 2$ and some N the optimal knots (with respect to $w(x) = (1-x)(1+x)$) and the sets D_2.

N	Knots	$D_2 \setminus \{-1,1\}$
4	$\pm$ 1	$[-\frac{1}{3}, \frac{1}{3}]$
	$\pm$ 0.44 721 360	

5	0 ± 1 ± 0.65 465 367	[− 0.61 596 253, − 0.11 596 253] [0.11 596 253, 0.61 596 253]
6	± 1 ± 0.76 505 532 ± 0.28 523 152	[− 0.74 821 804, − 0.38 166 834] [− 0.23 345 030, 0.23 345 030] [0.38 166 834, 0.74 821 804]
7	0 ± 1 ± 0.83 022 390 ± 0.46 884 879	[− 0.82 172 159, − 0.54 628 420] [− 0.44 212 448, − 0.05 089 521] [0.05 089 521, 0.44 212 448] [0.54 628 420, 0.82 172 159]
8	± 1 ± 0.95 179 510 ± 0.49 384 303 ± 0.21 019 670	[− 0.86 698 568, − 0.65 399 982] [− 0.57 652 878, − 0.25 499 676] [− 0.17 976 783, 0.17 976 783] [0.25 499 676, 0.57 652 878] [0.65 399 982, 0.86 698 568]

Here $|D_2| = 2\,\frac{N-3}{N-1}$ (cf. theorem 1 with $x_0 = -1$, $x_n = 1$).

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