

Evaluation of Taylor coefficients in Pade-Laplace method using cubic splines

Ibryaeva Olga

South Ural State University, Lenin avenue 76, Chelyabinsk, Russia, oli@6v6power.ru

A new method for the evaluation of the Taylor coefficients in the Pade-Laplace method is proposed. It is based on replacing a signal (with noise) in the integrals defining Taylor coefficients with its (smoothing) cubic spline. This makes possible to carry out integration exactly and avoid numerical integration errors. The proposed method gives more accurate results at some center points of Taylor series expansion compared to the trapezoidal rule and Simpson's rule.

I. INTRODUCTION

Multi-exponential signals $f(x) = \sum_{k=1}^N A_k e^{\mu_k x}$ (A_k , μ_k are complex) are found in such diverse areas as nuclear science, chemical kinetics, biomedicine, semiconductors, thermal responses, etc. Parameters A_k , μ_k are important monitoring parameters, because the fault occurring and development often cause the signal parameters change [1-3].

The Pade-Laplace method [4] based upon Padé approximants and the Laplace transform is one of the methods proposed for the analysis of these signals.

In paper [5] this method is applied to shear stress relaxation experiments performed with melt samples of polystyrene and polypropylene. The major interest of this method lies in the fact that it detects through its own stability the number of modes necessary to fit the signal without any assumption. In [6] the method is used for analyzing multiexponential decays to signal-averaged voltages obtained from a simple electronic circuit. In [7] the method is applied to the transient electric birefringence decay analysis. In [8] an insurance risk model is considered and an explicit expression for the distribution of probability of ultimate ruin, the expected time to ruin and the distribution of deficit at the time of ruin are derived using Pade-Laplace method.

Despite numerous works on this topic there are still many open challenges that need to be addressed. They are discussed in the next section. This paper is devoted to one of them – to the question of the Taylor coefficients evaluation in the Pade-Laplace method. A new method for their evaluation using cubic splines is proposed in Sect.3. An example of using this method is given in

Sect.4. It is shown that at some center points p_0 of the Taylor series expansion the proposed method gives more accurate results than the Trapezoidal rule and the Simpson's rule. The final section concludes this paper.

II. PADE-LAPLACE METHOD AND COMPUTATIONAL ASPECTS

The Pade-Laplace method allows to find the number N of exponentials and the parameters A_k , μ_k of the signal $f(x) = \sum_{k=1}^N A_k e^{\mu_k x}$ and it is based upon analytic continuation of the Laplace transform for $f(x)$ with a Pade approximant.

The Laplace transform for $f(x)$ is a rational function $L(p) = \int_0^{\infty} e^{-px} f(x) dx = \sum_{k=1}^N \frac{A_k}{p - \mu_k}$. Detecting the exponential components μ_k and the amplitudes A_k is then a matter of identifying the poles of $L(p)$ and the corresponding residues. This involves three steps. The first step is to express $L(p)$ at a specific point p_0 as a polynomial function through the use of a truncated Taylor expansion: $\sum_{r=0}^K c_r (p - p_0)^r$, $c_r = \frac{1}{r!} \frac{d^r L(p)}{dp^r} \Big|_{p=p_0}$,

$$\frac{d^r L(p)}{dp^r} = \int_0^{\infty} (-x)^r f(x) e^{-px} dt.$$

Given $L+M+1$ terms in the Taylor series, i.e. $K=L+M$, one can construct the type (M, L) Pade approximant in the second step of the Pade-Laplace

$$\text{method: } \pi_{L,M}(p) = \frac{\sum_{m=0}^M a_m (p - p_0)^m}{\sum_{l=0}^L b_l (p - p_0)^l}.$$

The coefficients a_k , b_l are derived from c_r . Since the function $L(p)$ is a rational function of degree $N-1$ for the numerator and N for the denominator, the Pade table for $L(p)$ has an infinite singular block, i.e. the Pade approximant $\pi_{N-1,N}(p)$ and all the type (M, L) Pade approximant with $M \geq N-1$, $L \geq N$ are equal to $L(p)$.

In order to determine the number N of modes, one

should consider the sequence of Pade approximants $\pi_{M-1,M}(p)$, $M = 2, 3, \dots$. If M is greater than N , then $\pi_{M-1,M}(p)$ has true poles μ_k , $k = 1, \dots, N$, and spurious poles ν_k , $k = 1, \dots, M - N$, which are also zeros of the numerator of $\pi_{M-1,M}(p)$. After canceling common factors, the Pade approximant $\pi_{M-1,M}(p)$ will be equal to $\pi_{N-1,N}(p)$. The third step of the method is to find the poles and residues of the Pade approximant.

There are some problems in practical use of the Pade-Laplace method. The spurious paired roots in the numerators and the denominators will not be rigorously equal. The phenomenon of pairing of such zeros and poles got the name of *Froissart phenomenon* and the pairs are known as *Froissart doublets* [9]. This problem was partially solved by the recent papers [10], [11] where new algorithms for computing Pade approximants which removes Froissart doublets induced by computer roundoff and by singular blocks in the Pade table were proposed.

Although theoretically the solution should not depend on p_0 , in practice the method may give an unstable solution if *the choice of p_0* is poor (see [7], [12] for details and some solutions to the problem). The value chosen for p_0 can significantly affect the numerical precision in the calculation of the integrals defining the coefficients c_r of the Taylor series expansion of $L(p)$. It is of importance, since Pade approximants are known to be very sensitive to errors in the coefficients.

In addition, the accuracy of c_r is directly related with the accuracy of numerical integration. Thus the third problem is *the choice of the numerical integration method* for the evaluation of Taylor coefficients of the Laplace transform. The most commonly used methods are the trapezoidal rule, Simpson's rule and the Gauss-Laguerre quadrature rule.

According to the Gauss-Laguerre integration method, the integral $\int_0^\infty e^{-x} F(x) dx$ is replaced by a finite sum $\sum_{j=1}^P w_j F(x_j)$, where x_j and w_j are respectively the abscissas and weights of the Gauss-Laguerre formula with P points. This method seems preferable if the function $F(x)$ is known, but in practice we have to integrate tabulated data rather than known functions and the integrand can not be evaluated for any desired abscissa value. The reasonable approach is to fit the data with a spline (or a smoothing spline if the data contain noise) and integrate formally.

In the next section a new method for evaluation of the Taylor coefficients using cubic splines is proposed. We will replace $f(x)$ by its cubic spline and obtain explicit formulas for the Taylor coefficients.

III. EVALUATION OF TAYLOR COEFFICIENTS USING CUBIC SPLINE

A. Cubic spline

Definition 1: Given n data points, $(x_1, y_1), \dots, (x_n, y_n)$. The function $S(x)$ is called a *cubic spline* if there exist $n-1$ cubic polynomials $S_i(x)$ with coefficients a_i, b_i, c_i, d_i that satisfy the following properties:

- I. $S(x) = S_i(x) = a_i + b_i(x - x_i) + c_i(x - x_i)^2 + d_i(x - x_i)^3$, for $x \in (x_i, x_{i+1})$, $i = 1, \dots, n-1$.
- II. $S(x_i) = y_i$, $i = 1, \dots, n$.
- III. $S_i(x_{i+1}) = S_{i+1}(x_{i+1})$, $i = 1, \dots, n-2$.
- IV. $S_i'(x_{i+1}) = S_{i+1}'(x_{i+1})$, $i = 1, \dots, n-2$.
- V. $S_i''(x_{i+1}) = S_{i+1}''(x_{i+1})$, $i = 1, \dots, n-2$.

Property I states that $S(x)$ consists of piecewise cubics. Property II states that the piecewise cubics interpolate the given set of data points. Properties III and IV require that the piecewise cubics represent a smooth continuous function. Property V states that the second derivative of the resulting function is also continuous.

The data points supply n conditions, and properties III, IV and V each supply $n-2$ conditions. Hence, $n + 3(n-2) = 4n - 6$ conditions are specified for $4(n-1)$ coefficients to be determined.

We can have different cubic splines depending on how we want to use our extra constraints. Here are some common ones:

1. $S_1''(x_1) = S_{n-1}''(x_n) = 0$ (the natural spline),
2. The user defines $S_1'(x_1)$ and $S_{n-1}'(x_n)$ (the clamped spline),
3. $S_1'''(x_2) = S_2'''(x_2)$, $S_{n-2}'''(x_{n-2}) = S_{n-1}'''(x_{n-2})$ (the not-a-knot spline).

Often, function values are perturbed by measurement errors. Matching such noisy data exactly results in unwanted oscillations. A standard remedy is to minimize a weighted sum of the squares of the interpolation errors in combination with the square integral of the second derivative to control the amount of smoothing.

Definition 2: Given n data points, $(x_1, y_1), \dots, (x_n, y_n)$. The function $S(x)$ is called a *smoothing cubic spline* if it:

- I. is a cubic polynomial $S(x) = S_i(x) = a_i + b_i(x - x_i) + c_i(x - x_i)^2 + d_i(x - x_i)^3$ on each partial segment (x_i, x_{i+1}) , $i = 1, \dots, n-1$,
- II. has the continuous second derivative on (x_1, x_n) ,
- III. minimizes the value of

$$L = p \sum_{i=1}^n w_i (y_i - S(x_i))^2 + (1-p) \int_{x_1}^{x_n} (S''(x))^2 dx,$$

where w_i are given numbers (weights).

The smoothing parameter $p \in [0,1]$ reflects the relative importance which we give to the conflicting objectives of remaining close to the data, on the one hand, and of obtaining a smooth curve, on the other hand.

B: Formulas for Taylor coefficients

Let us first state the following lemma.

Lemma: Let $S(x)$ be a 3rd degree polynomial and $P(x) = x^r S(x)$, where $r = 0,1,2,\dots$. Let p_0 does not equal to 0. Then

$$\begin{aligned} & \frac{P(x)}{p_0} + \frac{P'(x)}{p_0^2} + \frac{P''(x)}{p_0^3} + \dots + \frac{P^{(r+3)}(x)}{p_0^{r+4}} = \\ & = r! \sum_{k=0}^r \left(\frac{S(x)}{p_0} + \frac{(k+1)S'(x)}{p_0^2} + \frac{(k+2)(k+1)S''(x)}{2p_0^3} + \right. \\ & \left. + \frac{(k+3)(k+2)(k+1)S'''(x)}{6p_0^4} \right) \frac{x^{r-k}}{(r-k)!p_0^k}. \end{aligned}$$

Proof:

The statement is verified by directly computing all the derivatives and by using formulas $(x^r)^{(k)} = \frac{r!}{(r-k)!} x^{r-k}$, $k = 0, \dots, r$.

Now we can formulate the main result of this paper.

Theorem: Let $S(x)$ be a cubic spline (or a smoothing cubic spline) for $f(x)$. Replace $f(x)$ with $S(x)$ in the formulas for the Taylor coefficients c_r , $r = 0,1,\dots$:

$$c_r = \frac{(-1)^r}{r!} \int_0^\infty x^r f(x) e^{-p_0 x} dx \approx \frac{(-1)^r}{r!} \int_0^\infty x^r S(x) e^{-p_0 x} dx.$$

Then

$$\begin{aligned} & \frac{(-1)^r}{r!} \int_0^\infty x^r S(x) e^{-p_0 x} dx = (-1)^{r+1} \left\{ e^{-p_0 x_n} \sum_{k=0}^r \left(\frac{y_n}{p_0} + \right. \right. \\ & \left. \left. + \frac{(k+1)(b_{n-1} + 2c_{n-1}h_{n-1} + 3d_{n-1}h_{n-1}^2)}{p_0^2} + \right. \right. \\ & \left. \left. + \frac{(k+2)(k+1)(c_{n-1} + 3d_{n-1}h_{n-1})}{2p_0^3} + \right. \right. \\ & \left. \left. + \frac{(k+3)(k+2)(k+1)d_{n-1}}{p_0^4} \right) \frac{x_n^{r-k}}{(r-k)!p_0^k} + \right. \\ & \left. - e^{-p_0 x_1} \sum_{k=0}^r \left(\frac{y_1}{p_0} + \frac{(k+1)b_1}{p_0^2} + \frac{(k+2)(k+1)c_1}{p_0^3} + \right. \right. \end{aligned}$$

$$\begin{aligned} & \left. \left. + \frac{(k+3)(k+2)(k+1)d_1}{p_0^4} \right) \frac{x_1^{r-k}}{(r-k)!p_0^k} + \right. \\ & \left. + \sum_{i=2}^{n-1} e^{-p_0 x_i} (d_{i-1} - d_i) \sum_{k=0}^r \frac{(k+3)(k+2)(k+1)x_i^{r-k}}{(r-k)!p_0^{k+4}} \right\}. \end{aligned}$$

Here we denoted $x_n - x_{n-1}$ by h_{n-1} .

Proof: See Appendix A.

Remark 1: If $x_1 = 0$, the equation simplifies to

$$\begin{aligned} & \frac{(-1)^r}{r!} \int_0^\infty x^r S(x) e^{-p_0 x} dx = (-1)^{r+1} \left\{ e^{-p_0 x_n} \sum_{k=0}^r \left(\frac{y_n}{p_0} + \right. \right. \\ & \left. \left. + \frac{(k+1)(b_{n-1} + 2c_{n-1}h_{n-1} + 3d_{n-1}h_{n-1}^2)}{p_0^2} + \right. \right. \\ & \left. \left. + \frac{(k+2)(k+1)(c_{n-1} + 3d_{n-1}h_{n-1})}{2p_0^3} + \right. \right. \\ & \left. \left. + \frac{(k+3)(k+2)(k+1)d_{n-1}}{p_0^4} \right) \frac{x_n^{r-k}}{(r-k)!p_0^k} - \left(\frac{y_1}{p_0} + \frac{(r+1)b_1}{p_0^2} \right. \right. \\ & \left. \left. + \frac{(r+2)(r+1)c_1}{p_0^3} + \frac{(r+3)(r+2)(r+1)d_1}{p_0^4} \right) \frac{1}{p_0^r} + \right. \\ & \left. + \sum_{i=2}^{n-1} e^{-p_0 x_i} (d_{i-1} - d_i) \sum_{k=0}^r \frac{(k+3)(k+2)(k+1)x_i^{r-k}}{(r-k)!p_0^{k+4}} \right\}. \end{aligned}$$

Remark 2: It is easy to see that if $p_0 = 0$, then

$$\begin{aligned} c_r & = \frac{(-1)^r}{r!} \int_0^\infty x^r f(x) dx \approx \frac{(-1)^r}{r!} \int_0^\infty x^r S(x) dx = \\ & = (-1)^r \sum_{i=1}^{n-1} \sum_{k=0}^r \frac{x_i^{r-k} h_i^{k+1}}{(r-k)!k!} \left(\frac{y_i}{k+1} + \frac{b_i h_i}{k+2} + \frac{c_i h_i^2}{k+3} + \frac{d_i h_i^3}{k+4} \right). \end{aligned}$$

Here we denoted $x_{i+1} - x_i$ by h_i .

The next section contains an example, where the obtained formulas are used for the evaluation of the Taylor coefficients.

IV. AN EXAMPLE

Consider an exponentially damped sinusoidal signal $f(t) = e^{-0.1t} \cos t$ corrupted with white Gaussian noise (SNR=10dB), with a sampling frequency of 1 kHz and a signal duration of 10 seconds.

We fit the noisy signal with a cubic-smoothing spline using the Matlab function `csaps` with the smoothing parameter set to 0.8. The signal and its spline are shown in the figure 1.

Let us calculate the first twenty coefficients c_r of the Taylor series expansion of the Laplace transform of $f(t)$ at the point $p_0 = 500$. The trapezoidal rule, Simpson's rule and our method based on the smoothing cubic spline for $f(t)$ are used.

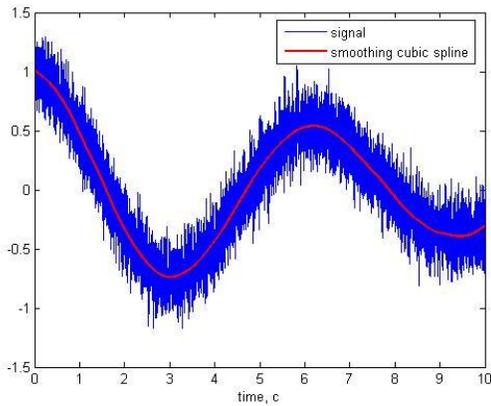


Fig 1. Cubic smoothing spline to noisy data

The results, along with the true values, are given in Table 1. In order to compare the results given by three considered methods, calculate the *percentage relative error*:

$$\delta_{meas} = \frac{|c_{true} - c_{meas}|}{|c_{true}|} \cdot 100\%.$$

Here c_{true} is the true value of the Taylor coefficient, c_{meas} is the value obtained by one of three considered methods.

The figure 2 shows the comparison between the methods.

Table 1. Taylor coefficients at $p_0 = 500$

True values	Our method with splines	Trapezoidal rule	Simpson's rule
1.9996e-003	2.0244e-003	1.8755e-003	1.8058e-003
-3.9984e-006	-4.0464e-006	-3.8567e-006	-3.9304e-006
7.9950e-009	8.0877e-009	8.2157e-009	8.3018e-009
-1.5987e-011	-1.6165e-011	-1.6703e-011	-1.6874e-011
3.1966e-014	3.2310e-014	3.3513e-014	3.3856e-014
-6.3918e-017	-6.4580e-017	-6.6884e-017	-6.7554e-017
1.2781e-019	1.2908e-019	1.3318e-019	1.3433e-019
-2.5555e-022	-2.5800e-022	-2.6485e-022	-2.6646e-022
5.1099e-025	5.1567e-025	5.2651e-025	5.2806e-025
-1.0217e-027	-1.0307e-027	-1.0473e-027	-1.0477e-027
2.0430e-030	2.0601e-030	2.0862e-030	2.0841e-030
-4.0849e-033	-4.1175e-033	-4.1626e-033	-4.1574e-033
8.1678e-036	8.2299e-036	8.3162e-036	8.3110e-036
-1.6331e-038	-1.6449e-038	-1.6624e-038	-1.6631e-038
3.2654e-041	3.2878e-041	3.3223e-041	3.3280e-041
-6.5291e-044	-6.5715e-044	-6.6342e-044	-6.6544e-044
1.3055e-046	1.3135e-046	1.3232e-046	1.3291e-046
-2.6102e-049	-2.6253e-049	-2.6364e-049	-2.6520e-049
5.2190e-052	5.2472e-052	5.2485e-052	5.2873e-052
-1.0435e-054	-1.0488e-054	-1.0446e-054	-1.0537e-054

As one can see, all methods give similarly low error but our method is more accurate than others.

The average mean $\bar{\delta}_{meas}$ of the relative error is 0.86 for the method with splines, 2.7 and 3.2 for the Trapezoidal rule and the Simpson's rule, respectively.

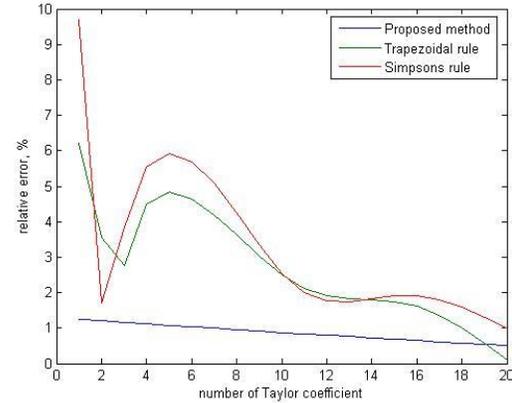


Fig.2 Relative errors of the Taylor coefficients calculated at the point $p_0 = 500$

It is worth mentioning that the accuracy of all these methods depends significantly on the choice of p_0 . Table 2 contains the Taylor coefficients calculated at $p_0 = 1$.

Table 2. Taylor coefficients at $p_0 = 1$

True values	Our method with splines	Trapezoidal rule	Simpson's rule
4.9774e-001	5.0268e-001	5.0261e-001	5.0285e-001
-4.2997e-002	-4.6152e-002	-4.6272e-002	-4.6129e-002
-1.8242e-00	-1.8038e-001	-1.8052e-001	-1.8058e-001
2.0105e-001	1.9933e-001	1.9978e-001	1.9954e-001
-1.1760e-001	-1.1558e-001	-1.1672e-001	-1.1619e-001
2.6092e-002	2.3433e-002	2.6016e-002	2.5268e-002
2.7237e-002	3.0498e-002	2.5492e-002	2.6350e-002
-3.8920e-002	-4.2329e-002	-3.3848e-002	-3.4716e-002
2.6420e-002	2.9340e-002	1.6510e-002	1.7302e-002
-8.6892e-003	-1.0808e-002	6.8527e-003	6.1949e-003
-3.3047e-003	-1.4810e-003	-2.3970e-002	-2.3467e-002
7.2215e-003	4.2417e-003	3.1119e-002	3.0761e-002
-5.6935e-003	4.6557e-004	-3.0067e-002	-2.9829e-002
2.4001e-003	-8.8469e-003	2.4498e-002	2.4347e-002
1.8703e-004	1.7677e-002	-1.7676e-002	-1.7586e-002
-1.2722e-003	-2.5106e-002	1.1586e-002	1.1535e-002
1.1818e-003	3.0523e-002	-7.0058e-003	-6.9776e-003
-6.0081e-004	-3.4073e-002	3.9485e-003	3.9337e-003
6.3334e-005	3.6206e-002	-2.0897e-003	-2.0822e-003
2.0881e-004	-3.7396e-002	1.0443e-003	1.0406e-003

The figure 3 shows the relative errors of the Taylor coefficients.

The notable difference between the true values and the calculated values once again stresses the importance of the parameter p_0 which must be chosen in an optimal interval.

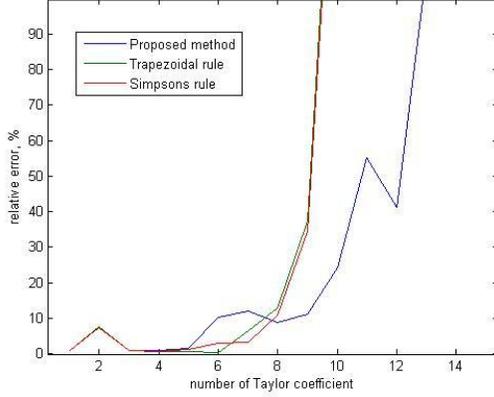


Fig.3 Relative errors of the Taylor coefficients calculated at the point $p_0 = 1$

Our further experiments showed that the proposed method gives (at least at some points p_0) more accurate results compared to the Trapezoidal rule and the Simpson's rule and, hence, can be used along with them.

V. CONCLUSIONS

The paper is devoted to one of the problems in the Pade-Laplace method, namely, the problem of the Taylor coefficients evaluation. These coefficients are used to construct Pade approximants in the Pade-Laplace method and their accurate evaluation is important since Pade approximants are known to be very sensitive to errors in the Taylor coefficients.

The new method based on fitting data (a signal) with its cubic spline is proposed and the explicit formulas for the Taylor coefficients are obtained. Numerical experiments show that the new method outperforms the existing methods at least at some center points p_0 of the Taylor series expansion and can be used along with them since the problem of optimal choice of p_0 is still open.

It is considered that the optimal choice for p_0 is such that the coefficients of the Taylor series are all of the same order of magnitude. It is clear that for keeping optimal accuracy in the computer calculations it is not advantageous to deal with very rapidly decreasing Taylor series coefficients. On the other hand, the example in Sect. 4 shows that the Taylor coefficients were calculated at $p_0 = 1$ less accurate (by all the methods) than the coefficients calculated at $p_0 = 500$ which decrease rapidly. The problem of the optimal choice of p_0 clearly deserves further investigation in future studies.

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APPENDIX A PROOF OF THEOREM

Using the definition for $S(x)$ we have

$$\frac{(-1)^r}{r!} \int_0^\infty x^r S(x) e^{-p_0 x} dx = \frac{(-1)^r}{r!} \sum_{i=1}^{n-1} \int_{x_i}^{x_{i+1}} x^r S_i(x) e^{-p_0 x} dx.$$

Let us denote by $P_i(x)$ the degree $r+3$ polynomial

$$x^r S_i(x). \text{ Then we have } \frac{(-1)^r}{r!} \sum_{i=1}^{n-1} \int_{x_i}^{x_{i+1}} x^r S_i(x) e^{-p_0 x} dx =$$

$$= \frac{(-1)^{r+1}}{r!} \sum_{i=1}^{n-1} e^{-p_0 x} \left(\frac{P_i(x)}{p_0} + \frac{P_i'(x)}{p_0^2} + \dots + \frac{P_i^{(r+3)}(x)}{p_0^{r+4}} \right) \Big|_{x_i}^{x_{i+1}}.$$

By making substitution and using Lemma, we obtain

$$\begin{aligned} & \frac{(-1)^{r+1}}{r!} \left\{ \sum_{i=1}^{n-1} e^{-p_0 x_{i+1}} r! \sum_{k=0}^r \left(\frac{S_i(x_{i+1})}{p_0} + \frac{(k+1)S_i'(x_{i+1})}{p_0^2} + \right. \right. \\ & \left. \left. + \frac{(k+2)(k+1)S_i''(x_{i+1})}{2p_0^3} + \frac{(k+3)(k+2)(k+1)S_i'''(x_{i+1})}{6p_0^4} \right) \times \right. \\ & \left. \frac{x_{i+1}^{r-k}}{(r-k)!p_0^k} - \sum_{i=1}^{n-1} e^{-p_0 x_i} r! \sum_{k=0}^r \left(\frac{S_i(x_i)}{p_0} + \frac{(k+1)S_i'(x_i)}{p_0^2} + \right. \right. \\ & \left. \left. + \frac{(k+2)(k+1)S_i''(x_i)}{2p_0^3} + \frac{(k+3)(k+2)(k+1)S_i'''(x_i)}{6p_0^4} \right) \times \right. \\ & \left. \frac{x_i^{r-k}}{(r-k)!p_0^k} \right\}. \end{aligned}$$

By replacing the summation index i with $i+1$ in the first sum of the equation, we get

$$\begin{aligned} & (-1)^{r+1} \left\{ e^{-p_0 x_n} \sum_{k=0}^r \frac{x_n^{r-k}}{(r-k)!p_0^k} \left(\frac{S_{n-1}(x_n)}{p_0} + \frac{(k+1)S_{n-1}'(x_n)}{p_0^2} + \right. \right. \\ & \left. \left. + \frac{(k+2)(k+1)S_{n-1}''(x_n)}{2p_0^3} + \frac{(k+3)(k+2)(k+1)S_{n-1}'''(x_n)}{6p_0^4} \right) - \right. \\ & \left. e^{-p_0 x_1} \sum_{k=0}^r \frac{x_1^{r-k}}{(r-k)!p_0^k} \left(\frac{S_1(x_1)}{p_0} + \frac{(k+1)S_1'(x_1)}{p_0^2} + \right. \right. \\ & \left. \left. + \frac{(k+2)(k+1)S_1''(x_1)}{2p_0^3} + \frac{(k+3)(k+2)(k+1)S_1'''(x_1)}{6p_0^4} \right) + \right. \\ & \left. + \sum_{i=2}^{n-1} e^{-p_0 x_i} \sum_{k=0}^r \frac{x_i^{r-k}}{(r-k)!p_0^k} \left(\frac{S_{i-1}(x_i) - S_i(x_i)}{p_0} + \right. \right. \\ & \left. \left. + \frac{(k+1)(S_{i-1}'(x_i) - S_i'(x_i))}{p_0^2} + \frac{(k+2)(k+1)(S_{i-1}''(x_i) - S_i''(x_i))}{2p_0^3} \right) \right\} \end{aligned}$$

$$+ \frac{(k+3)(k+2)(k+1)(S_{i-1}'''(x_i) - S_i'''(x_i))}{6p_0^4} \Bigg\}.$$

Taking into account the continuity conditions of the first and second derivatives of the spline and using again the definition for $S(x)$, we obtain the desired formula.

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