Studies in Nonlinear Sciences 6 (1): 10-16, 2021 ISSN 2221-3910 © IDOSI Publications, 2021 DOI: 10.5829/idosi.sns.2021.10.16

Lagrangian Interpolation Formula and Sylvester's Matrix Function

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Abstract: We exhibit an elementary deduction of the remainder term in the Lagrange's polynomial interpolation, with examples for two and three data points via explicit Green functions. In particular, it is deduced the corresponding error term for the finite Taylor series. Besides, we use the Faddeev-Sominsky algorithm to obtain the Lanczos expression for the resolvent of a matrix. Finally, the previous results allow construct the Sylvester's interpolating matrix formula.

Key words: Finite Taylor series - Interpolation by polynomials - Green's function - Characteristic polynomial -Leverrier-Takeno's procedure - Sylvester matrix formula - Cayley-Hamilton-Frobenius theorem -Faddeev-Sominsky's algorithm - Resolvent of a matrix

INTRODUCTION

If we have the data points $(x_j, f_j \equiv f(x_j))$, j = 1, 2, ..., n then the function f(x) can be approximated by a polynomial of degree n - 1 constructed via the Lagrangian interpolation [1-4]:

$$P_n(x) = \sum_{k=1}^n p_k(x) \cdot f_k, \qquad P_n(x_j) = f_j, \quad j = 1, ..., n,$$
(1)

With the fundamental polynomial:

$$F_n(x) = (x - x_1) (x - x_2) \cdots (x - x_n), \quad F_n(x_j) = 0, \quad \forall \ j,$$
(2)

Such that:

$$\varphi_k(x) = \frac{F_n(x)}{x - x_k}, \qquad \varphi_k(x_k) = F'_n(x_k), \qquad \varphi_k(x_j) = 0, \quad j \neq k,$$

$$p_k(x) = \frac{\varphi_k(x)}{\varphi_k(x_k)}, \qquad p_k(x_j) = \delta_{jk}.$$
(3)

The remainder term in this Lagrangian expansion is given by $\eta_n(x) = f(x) - P_n(x)$, satisfying a differential equation with boundary conditions [5]:

$$\eta_n^{(n)}(x) = f^{(n)}(x), \qquad \eta_n(x_j) = 0, \qquad j = 1, \dots, n,$$
(4)

Whose solution can be written in terms of the Green's function [6-11]:

$$\eta_n(x) = \int_{x_1}^{x_n} f^{(n)}(\xi) \cdot G(x,\xi) \, d\xi, \qquad \frac{d^n}{dx^n} G(x,\xi) = \delta(x-\xi), \qquad G(x_j,\xi) = 0, \quad \forall \ j.$$
(5)

The Rolle theorem applied to (5) allows obtain the following estimation:

$$\eta_n(x) = f^{(n)}(\bar{x}) \cdot \int_{x_1}^{x_n} G(x,\xi) \, d\xi, \qquad \bar{x} \, \varepsilon \, [x_1, \, x_n], \tag{6}$$

Thus the goal is to determine the function:

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$$g(x) = \int_{x_1}^{x_n} G(x,\xi) d\xi, \qquad g(x_j) = 0, \quad j = 1, \dots, n.$$
(7)

Here we give an elementary process to calculate explicitly the integral (7), which is verified with the corresponding Green functions for two and three data points. The polynomial (1) was obtained by Vandermonde (1771), Euler (1783), Waring (1779) and Lagrange (1795) [12, 13].

From (5) we see that $G^{(n)} = 0$ for $x \neq \xi$, then G is a polynomial of degree n - 1 in x and we know that (7) is applied in the form $g(x) = \int_{x_1}^x G_1 d\xi + \int_x^{x_n} G_2 d\xi$, therefore g(x) is a polynomial of degree n in x and the x_i are its roots, hence (7) has the structure:

$$g(x) = c (x - x_1) (x - x_2) \cdots (x - x_n),$$
(8)

and from (5), (7) and (8):

$$g^{(n)}(x) = \int_{x_1}^{x_n} G^{(n)} d\xi = \int_{x_1}^{x_n} \delta(x-\xi) d\xi = 1 = n! c,$$

That is:

$$\int_{x_1}^{x_n} G(x,\xi) \, d\xi = \frac{1}{n!} \, F_n(x), \tag{9}$$

Thus (6) and (9) imply the following expression for the remainder term of Lagrangian interpolation formula [2]:

$$\eta_n(x) = \frac{1}{n!} f^{(n)}(\bar{x}) F_n(x).$$
(10)

If n = 2 then the Green function verifying the properties (5) is given by:

$$G_{+} = \frac{1}{x_{2} - x_{1}} \left(\xi - x_{1}\right) \left(x - x_{2}\right), \quad x > \xi, \qquad \qquad G_{-} = \frac{1}{x_{2} - x_{1}} \left(x - x_{1}\right) \left(\xi - x_{2}\right), \quad x < \xi, \qquad (11)$$

Therefore:

$$\int_{x_1}^{x_2} G(x,\xi) d\xi = \int_{x_1}^x G_+ d\xi + \int_x^{x_2} G_- d\xi = \frac{1}{2} (x-x_1) (x-x_2),$$

in according with (9).

For n = 3 we must consider two regions with their corresponding Green function:

$$x_1 \leq \xi \leq x_2$$
:

$${}_{1}G_{-} = \frac{(x-x_{1})\left[(x-x_{3})(x_{3}-x_{1})(x_{2}-\xi)^{2}-(x-x_{2})(x_{2}-x_{1})(x_{3}-\xi)^{2}\right]}{2(x_{2}-x_{1})(x_{3}-x_{1})(x_{3}-x_{2})}, \quad x \leq \xi; \quad {}_{1}G_{+} = \frac{1}{2}(x-\xi)^{2} + {}_{1}G_{-}, \quad x \geq \xi,$$

$$x_{2} \leq \xi \leq x_{3}: \qquad (12)$$

$$x_2 \le \xi \le x_3:$$

$${}_{2}G_{-} = -\frac{(x-x_{1})(x-x_{2})(x_{3}-\xi)^{2}}{2(x_{3}-x_{1})(x_{3}-x_{2})}, \quad x \leq \xi; \qquad {}_{2}G_{+} = \frac{1}{2}(x-\xi)^{2} + {}_{2}G_{-}, \quad x \geq \xi,$$

and the verification of $\int_{x_1}^{x_n} G d\xi$ also is in two regions:

$$\begin{aligned} x_1 &\leq x \leq x_2: \quad \int_{x_1}^{x_3} G \, d\xi = \int_{x_1}^{x} {}_1G_+ \, d\xi + \int_{x}^{x_2} {}_1G_- \, d\xi + \int_{x_2}^{x_3} {}_2G_- \, d\xi = \frac{1}{3!} \, (x - x_1)(x - x_2)(x - x_3), \\ x_2 &\leq x \leq x_3: \quad \int_{x_1}^{x_3} G \, d\xi = \int_{x_1}^{x_2} {}_1G_+ \, d\xi + \int_{x_2}^{x} {}_2G_+ \, d\xi + \int_{x}^{x_3} {}_2G_- \, d\xi = \frac{1}{3!} \, F_3(x), \end{aligned}$$

In harmony with (9).

For the general case the Green function is given by [2]:

$${}_{j}G_{-} = -\frac{1}{(n-1)!} \sum_{k=j+1}^{n} p_{k}(x) (x_{k} - \xi)^{n-1}, \quad x \le \xi; \qquad {}_{j}G_{+} = \frac{1}{(n-1)!} (x - \xi)^{n-1} + {}_{j}G_{-}, \quad x \ge \xi,$$
(13)

for the intervals $x_j \le \xi \le x_{j+1}$, j = 1, 2, ..., n-1.

If we consider that the data points are equidistant and that they all collapse into $x_1 = a$, then (10) implies the remainder term for the finite Taylor expansion:

$$\eta_n(x) = \frac{1}{n!} f^{(n)}(\bar{x}) (x-a)^n, \qquad \bar{x} \in [a, x],$$
(14)

Thus the Lagrangian interpolation is transformed to Taylor extrapolation.

On the other hand, for an arbitrary matrix $\mathbf{A}_{nxn} = (\mathbf{A}_{i}^{i})$ its characteristic polynomial [1, 2, 14-16]:

$$p(\lambda) \equiv \lambda^n + a_1 \,\lambda^{n-1} + \dots + a_{n-1} \,\lambda + a_n \,, \tag{15}$$

Can be obtained through several procedures [1, 17-21]. The approach of Leverrier-Takeno [22-26] is a simple and interesting technique to construct (15) based in the traces of the powers \mathbf{A}^r , r = 1, ..., n. Besides, it is well known that an arbitrary matrix satisfies its characteristic equation, which is the Cayley-Hamilton-Frobenius identity [1, 2, 14-16, 27, 28]:

$$\mathbf{A}^{n} + a_{1} \, \mathbf{A}^{n-1} + \dots + a_{n-1} \, \mathbf{A} + a_{n} \, \mathbf{I} = \mathbf{0}.$$
 (16)

If A is non-singular (that is, det $A \neq 0$), then from (16) we obtain its inverse matrix:

$$\mathbf{A}^{-1} = -\frac{1}{a_n} (\mathbf{A}^{n-1} + a_1 \, \mathbf{A}^{n-2} + \dots + a_{n-1} \, \mathbf{I}), \tag{17}$$

where $a_n \neq 0$ because $a_n = (-1)^n \det \mathbf{A}$.

Faddeev-Sominsky [29-38] proposed an algorithm to determine A^{-1} in terms of A^r and their traces, which is equivalent [37] to the Cayley-Hamilton-Frobenius theorem (16) plus the Leverrier-Takeno's method to construct the characteristic polynomial of a matrix A. Here we employ the Faddeev-Sominsky's procedure to obtain the Lanczos expression [39] for the resolvent of A [34, 35, 40- 43], that is, the Laplace transform of exp(t A) [44].

If we define the quantities:

$$a_0 = 1, \quad s_k = tr \, \mathbf{A}^k, \quad k = 1, 2, \dots, n$$
 (18)

Then the process of Leverrier-Takeno [17, 22-26] implies (1) wherein the a_i are determined with the Newton's recurrence relation:

$$r a_r + s_1 a_{r-1} + s_2 a_{r-2} + \dots + s_{r-1} a_1 + s_r = 0, \quad r = 1, 2, \dots, n$$
(19)

Therefore:

$$a_{1} = -s_{1}, \quad 2! \ a_{2} = (s_{1})^{2} - s_{2}, \quad 3! \ a_{3} = -(s_{1})^{3} + 3 \ s_{1} \ s_{2} - 2 \ s_{3},$$

$$4! \ a_{4} = (s_{1})^{4} - 6 \ (s_{1})^{2} \ s_{2} + 8 \ s_{1} \ s_{3} + 3 \ (s_{2})^{2} - 6 \ s_{4}, \quad etc.$$

(20)

In particular, det $A = (-1)^n a_n$, that is, the determinant of any matrix only depends on the traces s_r , which means that A and its transpose have the same determinant. In [45, 46] we find the general expression:

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$$a_{k} = \frac{(-1)^{k}}{k!} \begin{vmatrix} s_{1} & k-1 & 0 & \cdots & 0 \\ s_{2} & s_{1} & k-2 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ s_{k-1} & s_{k-2} & \cdots & \cdots & 1 \\ s_{k} & s_{k-1} & \cdots & \cdots & s_{1} \end{vmatrix}, \qquad k = 1, \dots, n.$$
(21)

The Faddeev-Sominsky's procedure [29-38] to obtain A^{-1} is a sequence of algebraic computations on the powers A^r and their traces, in fact, this algorithm is given via the instructions:

$$B_{1} = A, \qquad q_{1} = \operatorname{tr} B_{1}, \qquad C_{1} = B_{1} - q_{1} I,$$

$$B_{2} = C_{1} A, \qquad q_{2} = \frac{1}{2} \operatorname{tr} B_{2}, \qquad C_{2} = B_{2} - q_{2} I,$$

$$\vdots \qquad \vdots \qquad \vdots \qquad \vdots$$

$$B_{n-1} = C_{n-2} A, \qquad q_{n-1} = \frac{1}{n-1} \operatorname{tr} B_{n-1}, \qquad C_{n-1} = B_{n-1} - q_{n-1} I,$$

$$B_{n} = C_{n-1} A, \qquad q_{n} = \frac{1}{n} \operatorname{tr} B_{n},$$

$$A^{-1} = \frac{1}{q_{n}} C_{n-1}.$$
(23)

Then:

For example, if we apply (22) for
$$n = 4$$
, then it is easy to see that the corresponding q_r imply (20) with $q_j = -a_j$, and besides (23) reproduces (17). By mathematical induction one can prove that (22) and (23) are equivalent to (17), (18) and (19), showing [37] thus that the Faddeev-Sominsky's technique has its origin in the Leverrier-Takeno method plus the Cayley-Hamilton-Frobenius theorem.

From (22) we can see that [41]:

$$\mathbf{C}_{k} = \mathbf{A}^{k} + a_{1}\mathbf{A}^{k-1} + a_{2}\mathbf{A}^{k-2} + \dots + a_{k-1}\mathbf{A} + a_{k}\mathbf{I}, \quad k = 1, 2, \dots, n-1, \quad \mathbf{C}_{n} = \mathbf{B}_{n} - q_{n}\mathbf{I} = \mathbf{0}, \quad (24)$$

and for k = n - 1:

$$\mathbf{C}_{n-1} = \mathbf{A}^{n-1} + a_1 \, \mathbf{A}^{n-2} + a_2 \, \mathbf{A}^{n-3} + \dots + a_{n-2} \, \mathbf{A} + a_{n-1} \, \mathbf{I} = -a_n \, \mathbf{A}^{-1}$$

In harmony with (23) because $a_n = -q_n$. The property $\mathbf{C}_n = \mathbf{0}$ is equivalent to (16); if **A** is singular, the process (22) gives the adjoint matrix of **A** [14-16, 30], in fact, $adj \mathbf{A} = (-1)^{n+1} \mathbf{C}_{n-1}$.

If the roots of (15) have distinct values, then the Faddeev-Sominsky's algorithm allows obtain the corresponding eigenvectors of **A** [19]:

$$\mathbf{A}\,\vec{u}_k = \lambda_k\,\vec{u}_k\,,\qquad k = 1, 2, \dots, n,\tag{25}$$

Because for a given value of k, each column of:

$$\mathbf{Q}_k \equiv \lambda_k^{n-1} \mathbf{I} + \lambda_k^{n-2} \mathbf{C}_1 + \dots + \mathbf{C}_{n-1} , \qquad (26)$$

Satisfies (25) [30, 32, 41], and therefore all columns of \mathbf{Q}_k are proportional to each other, that is, rank $\mathbf{Q}_k = 1$ [32]; we note that $\mathbf{Q}_k = \mathbf{Q}(\lambda_k)$ with the participation of the matrix:

$$\mathbf{Q}(z) \equiv z^{n-1} \mathbf{I} + z^{n-2} \mathbf{C}_1 + z^{n-3} \mathbf{C}_2 + \dots + z \mathbf{C}_{n-2} + \mathbf{C}_{n-1} .$$
(27)

By synthetic division of two polynomials [1]:

$$\frac{p(z)}{z-\lambda} = \sum_{r=0}^{n-1} (\lambda^r + a_1 \lambda^{r-1} + a_2 \lambda^{r-2} + \dots + a_{r-1} \lambda + a_r) z^{n-1-r}$$

Then under the change $\lambda \rightarrow \mathbf{A}$ we obtain the Lanczos expression for the resolvent of a matrix [34, 35, 39-44]:

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$$\frac{1}{z\,\mathbf{I}-\mathbf{A}} = \frac{1}{p(z)} \sum_{r=0}^{n-1} z^{n-1-r} \,\mathbf{C}_r = \frac{\mathbf{Q}(z)}{p(z)} \,; \tag{28}$$

If **A** is non-singular, then (28) for z = 0 implies (23). McCarthy [27] used (28) and the Cauchy's integral theorem in complex variable to show the Cayley-Hamilton-Frobenius identity indicated in (16); the relation (28) is the Laplace transform of exp(t **A**) [44].

On the other hand, Sylvester [47-51] obtained the following interpolating definition of $f(\mathbf{A})$:

$$f(\mathbf{A}) = \sum_{j=1}^{n} f(\lambda_j) \prod_{k \neq j} \frac{\mathbf{A} - \lambda_k \mathbf{I}}{\lambda_j - \lambda_k},$$
(29)

Which is valid if all eigenvalues are different from each other. Buchheim [52] generalized (29) to multiple proper values using Hermite interpolation [53], thereby giving the first completely general definition of a matrix function. From (28) and (29) for $f(s) = \frac{1}{z-s}$ we deduce the properties:

$$\mathbf{Q}(z) = \sum_{j=1}^{n} \prod_{k=1, \ k\neq j}^{n} \frac{z - \lambda_{k}}{\lambda_{j} - \lambda_{k}} \left(\mathbf{A} - \lambda_{k} \mathbf{I} \right) \qquad \therefore \qquad \mathbf{Q}_{j} = \prod_{k=1, \ k\neq j}^{n} \left(\mathbf{A} - \lambda_{k} \mathbf{I} \right),$$

$$\mathbf{Q}_{j} \vec{u}_{j} = \prod_{k=1, \ k\neq j}^{n} \left(\lambda_{j} - \lambda_{k} \right) \vec{u}_{j},$$
(30)

Hence the eigenvectors of **A** showed in (25) also are proper vectors of the matrices \mathbf{Q}_j . Besides, from (25) and (30):

$$\mathbf{A} \, \mathbf{Q}_j \, \vec{u}_j = \prod_{k=1, \ k \neq j}^n \, (\lambda_j - \lambda_k) \, \lambda_j \, \vec{u}_j = \lambda_j \, \mathbf{Q}_j \, \vec{u}_j \qquad \therefore \qquad \mathbf{A} \, \mathbf{Q}_j = \lambda_j \, \mathbf{Q}_j \,, \tag{31}$$

That is, each column of \mathbf{Q}_j is eigenvector of \mathbf{A} with proper value λ_j . The resolvent (28) implies the relation $(\mathbf{A} - z \mathbf{I}) \mathbf{Q}(z) = -p(z) \mathbf{I}$, then $(\mathbf{A} - \lambda_k \mathbf{I}) \mathbf{Q}(\lambda_k) = -p(\lambda_k) \mathbf{I} = \mathbf{0}$ in according with (31).

From the Sylvester's formula (29) with f(z) = p(z) we obtain $p(\mathbf{A}) = \mathbf{0}$, which is the Cayley-Hamilton-Frobenius theorem indicated in (16). If $f(z) = e^{tz}$, then (29) allows to construct exp ($t\mathbf{A}$) [49, 54-56] that, in particular, is valuable to determine el motion of classical charged particles into a homogeneous electromagnetic field, and to integrate the Frenet-Serret equations with constant curvatures [57]. In [50, 58] we find that the book of Frazer-Duncan-Collar [40] emphasizes the important role of the matrix exponential in solving differential equations and was the first to employ matrices as an engineering tool, and indeed the first book to treat matrices as a branch of applied mathematics.

If we make the connections $x \to A_{nxn}$ and $x_j \to \lambda_j$, then from (1):

$$P_n(A) = \sum_{j=1}^n f(\lambda_j) \ p_j(A), \qquad p_j(A) = \prod_{k=1, \ k \neq j}^n \frac{A - \lambda_k I}{\lambda_j - \lambda_k}, \tag{32}$$

with the fundamental polynomial (2):

$$F_n(A) = (A - \lambda_1 I)(A - \lambda_2 I) \cdots (A - \lambda_n I) = 0,$$
(33)

where the Cayley-Hamilton-Frobenius (16) was applied; then from (10) is zero the remainder term of Lagrange's polynomial expansion, that is, $\eta_n(A) = 0$, therefore $f(A) = P_n(A)$ and thus (32) coincides with the Sylvester's expression (29), q.e.d. The properties (28) and (29) imply the relationship:

$$p_j(A) = \lim_{z \to \lambda_j} \frac{z - \lambda_j}{z \, l - A}.$$
(34)

The Sylvester's formula (29) is applicable for multiple eigenvalues if we employ adequately the Hopital-Bernoulli rule.

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