Tutorial for the seminar:

An introduction to Gauss quadrature and some extensions held at the *Università degli Studi di Pavia - Dipartimento di Meccanica Strutturale*

Author: **Francesco Calabrò** from *Università di Cassino, DAEIMI & Laboratorio di Analisi Numerica* - calabro@unicas.it

Starting point (!!):
Gauss, C. F. "Methodus nova integralium valores per approximationem inveniendi." Commentationes Societatis regiae scientarium Gottingensis recentiores 3, 39-76, 1814.

1 Definitions

Quadrature

Mathematical problem: Known $a, b \in \mathbb{R}$ and $f(x) : [a, b] \to \mathbb{R}$ calculate:

$$I(f) \equiv \int_a^b f(x)\,dx$$

Numerical problem: Choose n distinct points $x_i \in [a, b]$ (nodes) and relative coefficients $w_i \in \mathbb{R}$ (weights) such that:

$$\mathbb{I}_n(f) \equiv \sum_{i=1}^{n} w_i f(x_i) \approxeq I(f)$$

This means:

1. approximate the linear operator I by the quadrature rule $\mathbb{I}_n$;
2. approximate the measure dx by a finite combination of Diracs' delta: $dx \approx \sum_i w_i d\delta_{x_i}$.

With no constrains, how we choose nodes and weights? Consider now to know (or know how to calculate) the following:

$$M_j \equiv I(\phi_j(x)) = \int_a^b \phi_j(x) dx \quad \text{[Modified Moments]}$$

for some choice of functions $\phi_j(x)$.Then we can require that:

$$\sum_i w_i \phi_j(x_i) = M_j \qquad \forall j = 1, \ldots \qquad \text{(exactness equations)}$$

This is equivalent to require that the approximating measure solves the (modified) moment problem. Notice that if the previous holds true $\forall j = 1 \ldots m$ then we have, by linearity, that:

$$I(a_1\phi_1(x) + \cdots + a_m\phi_m(x)) = \mathbb{I}_n(a_1\phi_1(x) + \cdots + a_m\phi_m(x))$$
$$\forall a_j \in \mathbb{R}$$

thus the integration formula is exact for all the generalized polynomials.

2 Exactness

In the usual case, exactness is required with respect to polynomials. This is done by the following definition:

Definition, degree of exactness
We will call degree of exactness of the formula $\mathbb{I}_n$ the greatest positive integer r such that:

$$\int_a^b x^q \, d\mu_\alpha - \mathbb{I}_n(x^q) = 0 \qquad \forall\, 0 \le q \le r\,.$$

(We are taking in the previous as functions $\phi_j(x)$ the monomials x^{j-1}, and thus considering ordinary moments). It is well known that every quadrature rule with n nodes of degree of exactness at least $n-1$ is based on interpolation.

Theorem 1. *The quadrature rule $\mathbb{I}_n$ has degree of exactness $d = n - 1 + k$, $k \ge 0$ if and only if both of the following conditions are satisfied:*

1. *the formula integrates exactly is the (unique) polynomial of degree n interpolating the function f at the nodes x_i;*
2. *the following orthogonality property holds true:*

$$\int_a^b \omega_n(x) p(x) dx = 0 \quad \forall\, p \in \mathcal{P}^{k-1} \quad (\mathcal{P}^{-1} \equiv \emptyset) \tag{1}$$

where $\omega_n(x) \equiv \prod_{j=1}^n (x - x_i)$ (nodal polynomial)

($\mathcal{P}^k$ is the space of polynomials of degree k)

In the proof of the previous result the necessity is trivial, because both the interpolating polynomial and the product $\omega(x)p(x)$ are polynomials, and the second vanishes on the quadrature nodes. For sufficiency, consider to take $q(x) \in \mathcal{P}^{n-1+k}$ and write $q(x) = r_1(x)\omega(x) + r_2(x)$ with $r_1(x) \in \mathcal{P}^{k-1}, r_2(x) \in \mathcal{P}^{n-1}$. Now:

$$\int_a^b q(x)dx = \int_a^b \omega_n(x) r_1(x) dx + \int_a^b r_2(x) dx = \int_a^b r_2(x) dx = \tag{2}$$

now, since $r_2(x) \in \mathcal{P}^{n-1}$ the quadrature formula is exact, and thus:

$$\sum_{i=1}^n w_i r_2(x_i) = \sum_{i=1}^n w_i [q(x_i) - r_1(x_i)\omega_n(x_i)] = \sum_{i=1}^n w_i q(x_i) \tag{3}$$

where the last holds true because the nodal polynomial vanishes on the quadrature nodes. This completes the proof.

Observe that if the construction of a quadrature rule is made in a reference interval the rule that achieves the same degree of exactness in a general interval is obtained simply rescaling linearly the nodes and multiplying the weights by the measure of the interval. For this reason we will often refer ourselves to some special case, say $[0, 1]$ or $[-1, 1]$.

This is the theorem that permits to construct the quadrature rules. First, consider to know the nodes of the quadrature rule and call:

$$\mathcal{L}_i(x) = \left(\prod_{p=1;\, p\neq i}^{n} \frac{x - x_p}{x_i - x_p} \right) , \quad \Pi_n(x) = \sum_{i=1}^{n} f(x_i)\mathcal{L}_i(x)$$

$$\mathcal{L}_i(x) \, , \, \Pi_n(x) \in \mathcal{P}^{n-1} \, ,$$

the interpolating polynomial in the Lagrange form.

With this notation, from the theorem we have:

1. Weights of quadrature rules of degree of exactness $\geq n-1$ can be calculated as integrals of the Lagrange fundamental polynomials:

$$w_i = \int_a^b \mathcal{L}_i(x)\, dx$$

2. From the interpolation error, a simple error estimate con be derived:

$$\int_a^b f(x)\, dx - \mathbb{I}_n f = \int_a^b f(x)\, dx - \int_a^b \Pi_n(x)\, dx =$$

$$= \int_a^b \left[f(x) - \Pi_n(x) \right] \, dx = \frac{1}{n!} \int_a^b f^{(n)}(\xi_x)\omega_n(x)\, dx$$

The best that we can try to achieve in the Theorem is $k = n$. This is trivial, because the condition (1) for $k = n + 1$ would imply that $\omega_n(x)$ is orthogonal to all polynomials of degree n, and in particular to itself.

Gauss Rules, degree of exacness $= 2n - 1$
Optimal rules (from the degree of exactness point of view) are referred as Gauss quadrature rules. We will denote the unique Gauss rule on n point by $\mathbb{G}_n$.

Before considering how to construct this rules, we will notice some important features of gaussian quadrature.

Let us see that Gauss rules have positive weights. As before, call $\mathcal{L}$ the Lagrange fundamental polynomials, we have $\mathcal{L}_i(\xi_j) = \delta_{ij}$ and $\mathcal{L}_i \in \mathcal{P}^{n-1}$. Now observe that

$$\int_a^b \mathcal{L}_i^2(x)\, dx > 0 \, .$$

By the other side the rule is exact on the polynomials $\mathcal{L}_i^2(x) \in \mathcal{P}^{2n-2}$:

$$\int_a^b \mathcal{L}_i^2(x)\, d\mu(x) = \mathbb{G}_n(\mathcal{L}_i^2) = \sum_{j=1}^{n} w_j \mathcal{L}_i^2(\xi_j) = w_i \, ,$$

and thus the weights are positive, as requested.

Gauss quadrature is equivalent to exact integration of a particular interpolating polynomial.

Let us introduce the elementary Hermite interpolation polynomials (or Hermite characteristic polynomials):

$$\begin{cases} h_i(\xi_j) = \delta_{ij} \\ h_i'(\xi_j) = 0 \end{cases} \qquad \begin{cases} k_i(\xi_j) = 0 \\ k_i'(\xi_j) = \delta_{ij} \end{cases} \quad h_i(x), k_i(x) \in \mathcal{P}^{2n-1} \ \forall i = 1, \ldots, n$$

The Hemite-Birkoff polynomial is defined by: $\Pi_n^H(x) = \sum_{i=1}^n h_i(x) f(\xi_i) + k_i(x) f'(\xi_i)$. It interpolates the values of the function on nodes ξ again with the values of the derivatives on the same nodes.

Due to the fact that the Gauss quadrature integrates exactly op to degree $2n-1$ we obtain:

$$\int_a^b f(x)\,dx - \mathbb{G}_n f = \int_a^b f(x)\,dx - \int_a^b \Pi_n^H(x)\,dx = \int_a^b \left[f(x) - \Pi_n^H(x)\right]\,dx =$$

$$= \frac{1}{2n!}\int_a^b f^{(2n)}(\zeta_x)\omega_n^2(x)\,dx = \frac{f^{(2n)}(\zeta)}{2n!}\int_a^b \omega_n^2(x)\,dx$$

We can also write a characterization of Gauss quadrature in terms of the elementary Hermite polynomials.

Theorem 2. *The points ξ_i are nodes of a Gaussian rule iff*

$$\mathcal{F}_i = 0 \ \forall i = 1, \ldots, n \quad \textit{where } \mathcal{F}_i = \int_a^b k_i(x)\,dx\,.$$

The calculation of Gauss quadrature rule from this property is in principle possible, ma it is very expensive, due to the necessity to solve iteratively the interpolation problem for functions k_i. Details can be found in: J. Ma, V. Rokhlin, and S.Wandzura, Generalized Gaussian quadrature rules for systems of arbitrary functions, SIAM J. Numer. Anal. 33 (1996), no. 3, 971–996.

Also form the nonlinear map

$$\mathcal{G} : \mathbb{R}^{2n} \to \mathbb{R}^{2n}\,, \quad \mathcal{G}_j(x_1, \ldots, x_n, w_1, \ldots, w_n) = \left[\sum_{i=1}^n w_i (x_i)^{j-1}\right] - M_j$$

we can define a procedure for the calculation of the formulae. This because:

1. A quadrature rule is gaussian if and only if $\mathcal{G}_j = 0\,,\ \forall j = 1, \ldots, 2n$;
2. The map $\underline{\mathcal{G}}$ is always invertible

The calculation of the zero of this functional cen be done with a Newton (or some other of greater order) method but the Jacobian matrix is ill-conditioned, and also this method turns out to be not favorable.

3 Construction via orthogonal polynomials

Construction of the rules

As seen, the weights are fixed once the nodes are known.

From the theorem, we need to construct the nodes in such a way that the corresponding nodal polynomial respects an orthogonality property.

This can be done orthogonalizing the powers x^j with respect to the inner product $\langle u(x), v(x)\rangle = \int_a^b u(x)v(x)\,dx$.

The procedure is the following. Fix $\pi_0(x) = 1$. For all $j \geq 1$ find $\pi_j(x)$ a monic polynomial of degree exactly j such that $\int_a^b \pi_j(x)\pi_k(x)\,dx = 0\ \forall k < j$.

This is always possible because it is equivalent to the orthogonalization of Gram Schmidt of the consecutive powers.

This construction, in the case of the Lebesgue measure in a compact interval, leads to the so called Legendre orthogonal polynomials.

The important property is that:

Theorem 3. *All zeros of $\pi_n(x)$ are real, simple, and located in the interior of the support interval $[a, b]$.*

Proof Since $\int_a^b \pi_n(x)dx = 0$, there must exist at least one point in the interior of $[a, b]$ at which $\pi_n(x)$ changes sign. Let $x_1, x_2, \ldots, x_k\,, k \leq n$, be all such points. If we had $k < n$, then by orthogonality

$$\int_a^b \pi_n(x) \prod_{j=1}^{k} (x - x_j)dx = 0.$$

This, however, is impossible since the integrand has constant sign. Therefore, $k = n$.

From this property we can conclude that the nodes of the Gauss n-point quadrature rule are exactly the zeros of the orthogonal polynomial $\pi_n(x)$.

There are mainly two approaches in order to calculate the zeros of the polynomial $\pi_n(x)$.

The first one passes through the three term relation and is of algebraic type. The algorithm is due to Golub and Welsch, This is the method implemented in all numerical codes.

Main Reference
Golub & Welsch, "Calculation of Gauss quadrature rules" Math. Comp., v. 23, 1969, 221-230.

The second, very recent and powerful, uses the fact that the Legendre polynomials (in fact all the Jacobi ones) satisfy a Strum Liouville problem.

Main Reference
Glaser, Liu & Rokhlin, "A fast algorithm for the calculation of the roots of special functions" SIAM Journal on Scientific Computing, 2007.

Three term recursion

In order to construct the three term relation, we notice that the polynomials $\{\pi_k\}_{k=0,\dots,n}$ are a basis for the space $\mathcal{P}^n$ and, moreover, because π_{n+1} is monic, we have:

$$\pi_{n+1}(x) - x\pi_n(x) = -\alpha_n \pi_n(x) - \beta_n \pi_{n-1}(x) + \sum_{k=0}^{n-2} \gamma_{k,n} \pi_k(x)$$

From this equation, taking on both sides the scalar product with $\pi_n(x)$ first and $\pi_{n-1}(x)$ then we get the following expressions for α_n and β_n:

$$\alpha_n = \frac{\langle x\pi_n(x), \pi_n(x)\rangle}{\langle \pi_n(x), \pi_n(x)\rangle}\ ,\ n = 0, 1, \dots \ \beta_n = \frac{\langle \pi_n(x), \pi_n(x)\rangle}{\langle \pi_{n-1}(x), \pi_{n-1}(x)\rangle}\ ,\ n = 1, 2, \dots$$

Moreover taking the scalar product with $\pi_k(x)$ for $k \le n-2$ gives $\gamma_{k,n} = 0$.

From the first n of these coefficients we can construct the following tridiagonal matrix:

$$T \equiv \begin{bmatrix} \alpha_0 & 1 & & & 0 & \\ \beta_1 & \alpha_1 & 1 & & & \\ & \beta_2 & \ddots & \ddots & & \\ & & \ddots & \ddots & \ddots & \\ & & & \ddots & \ddots & 1 \\ & 0 & & & \beta_{n-1} & \alpha_{n-1} \end{bmatrix}$$

The three term relation for polynomials $\pi(x)$ written in matrix form reads:

$$x\underline{\pi}(x) = T\underline{\pi}(x) + \alpha_n \underline{e}_n \pi_n(x)$$

where $\underline{e}_n \in \mathbb{R}^{n\times 1}$, $\underline{e}_n = (0, \dots, 0, 1)$.

Hence, if ξ_i is a zero of $\pi_n(x)$, there follows $\xi_i\underline{\pi}(\xi_i) = T\underline{\pi}(\xi_i)$, and the eigenvalues of T are the requested quadrature nodes.

Making use of the Christoffel Darboux identity and the fact that $\pi_n(\xi_i) = 0$, the Gaussian weights are then expressed in terms of the eigenvectors of the Jacobian matrix. In particular, the weights can be computed from the first component of the orthonormal eigenvectors of T.

In the case of Legendre polynomials the coefficients α_i, β_i are known in closed form. In the case $[a, b] = [-1, 1]$ we have:

$$\alpha_i = 0\ \forall i \ge 0\ ,\ \beta_i = (4 - i^{-2})^{-1}\ \forall i \ge 1$$

Usually, for computational purpose, the following symmetric tridiagonal matrix (usually refereed to as Jacobi matrix) is considered instead:

$$J_n \equiv \begin{bmatrix} \alpha_0 & \sqrt{\beta_1} & & & 0 & \\ \sqrt{\beta_1} & \alpha_1 & \sqrt{\beta_2} & & & \\ & \sqrt{\beta_2} & \ddots & \ddots & & \\ & & \ddots & \ddots & \ddots & \\ & & & \ddots & \ddots & \sqrt{\beta_{n-1}} \\ & 0 & & & \sqrt{\beta_{n-1}} & \alpha_{n-1} \end{bmatrix}$$

This is due to the fact that it is diagonally similar to the previous and the computation of it's eigenvalues is simpler. Notice that the matrix identity $x\underline{\tilde{\pi}}(x) = J_n\underline{\tilde{\pi}}(x) + \alpha_n \underline{e}_n \tilde{\pi}_n(x)$ defines the orthonormal (not monic) version of the polynomials $\pi_i(x)$.

The calculation of the integral with Gauss quadrature rule, finally, reduces to:

- `function I = gauss(f,n)`
- $beta = \frac{1}{\sqrt{1-(2*[1:n-1])**(-2)}}$
- $J = diag(beta, 1) + diag(beta, -1);$
- `[V,D] = eig(J)`
- `x = diag(D); [x,i] = sort(x);`
- $w = 2 * V(1, i) * *2$
- $I = w * feval(f, x);$

This procedure is numerically stable and costs $o(n^2)$ operations.

Sketch of second method for the calculation of the zeros of orthogonal polynomials

The Legendre orthogonal polynomial $\pi_n(x)$ can be defined as the common polynomial solutions of the differential equation:

$$(1 - x^2)\frac{d^2\pi_n}{dx^2}(x) - 2x\frac{d\pi_n}{dx}(x) + n(n + 1)\pi_n(x) = 0,$$

The proposed method takes two steps to find each root. In the first step, an approximation to the root is found via a well-known analytical approximation. In the second step, the root is found via the Newton method, coupled with a Taylor series-based scheme for the solution of the original ODE equation.

Preliminary Definitions In the general case, we want to consider integration with respect to a general measure μ:

$$\int f \, d\mu$$

The only hypothesis for the measure μ that we need is that $\Lambda : \mathbb{R} \to \mathbb{R}\,,\ \Lambda(t) \equiv \int_{-\infty}^{t} d\mu$ is nondecreasing with at least n points of increase.

Notice that this hypothesis includes the weighted measures $d\mu = \omega(x)dx$ with $\omega(x)$ integrable nonnegative and non identically zero.

Moreover, we consider that the measure μ admits the modified moments defined by:

$$M_i \equiv \int_{-\infty}^{+\infty} \phi_i(x) \, d\mu \,,\ \forall i = 1, \ldots, 2n \,.$$

On the system of functions $\{\phi_i(x)\}_i \,,\ i = 1, \ldots, 2n$ we will have that the most general result on existence (but no uniqueness) of Gauss quadrature formulae is in:

Reference

Micchelli, C. A. and Pinkus, A. ”Moment theory for weak Chebyshev systems with applications to Monospolines, quadrature formulae and best one sided L-approximation by Spline functions with fixed knots”, SIAM J. MATH. ANAL. Vol. 8, No. 2, April 1977

4 Existence of Gauss Quadrature

4.1 Chebychev Systems

We will say that $\{\phi_i(x)\}_{j=1,\dots,m}$ form a Weak Chebyshev System if contains at least one strictly positive function and the following holds true:

$$\begin{vmatrix} \phi_1(x_1) & \phi_1(x_2) & \dots & \phi_1(x_m) \\ \phi_2(x_1) & \phi_2(x_2) & \dots & \phi_2(x_m) \\ \vdots & \vdots & \dots & \vdots \\ \phi_m(x_1) & \phi_m(x_2) & \dots & \phi_m(x_m) \end{vmatrix} \geq 0$$

$$\forall x_j \; s.t., \; j = 1, \dots, m \; a \leq x_1 < x_2 < \dots < x_m \leq b \, .$$

If $\{\phi_i(x)\}_{i=1,\dots,2n}$ form a weak Chebyshev system and μ is in the hypothesis seen previously we have that there exists a choice of points $\xi_i \, , \; i = 1, \dots, n \, , \; a \leq \xi_1 < \xi_2 < \dots < \xi_n \leq b$ and of weights $w_i \, , \; i = 1, \dots, n \, , \; w_i \geq 0$ such that:

$$\sum_{i=1}^{n} w_i \phi_j(\xi_i) = \int \phi_j \, d\mu \, , \; \forall j = 1, \dots, 2n \, .$$

We will call this quadrature rule Generalized Gauss formula.

If the previous determinant condition is satisfied with the strict inequality the family of functions $\{\phi_j(x)\}$ is sayed Chebyshev (or Haar) system and again with the existence of the gaussian quadrature we can prove uniqueness.

The important property of Chebychev systems is the following:

Theorem 4. *If $\{\phi_i(x)\}_{i=1,\dots,m}$ is a Chebyshev system in I then:*

1. *each $\Phi(x) = \sum_{i=1}^{m} a_i \phi_i(x)$ has at most $m - 1$ distinct zeros in I;*
2. *if $x_1, \dots, x_m$ are distinct points of I and $f_1, \dots, f_m$ are arbitrary numbers, then there exists a unique choice of the coefficients a_i such that $\sum_{i=1}^{m} a_i \phi_i(x_j) = f_j \, , \; \forall j = 1, \dots, m$.*

Examples of Chebyshev systems are:

- Spline - The $l + r$ functions:

  $$u_i(x) = x^{i-1} \; i = 1, \dots, l \, ; \; u_{l+j}(x) = \left(x - y_j\right)_+^{l-1} \; j = 1, \dots, r$$

  where

  $$y_+^p = \begin{cases} y^p & if \; x \geq 0 \\ 0 & if \; x < 0 \end{cases}$$

  and y_j are distinct (fixed) points $\in (-1, 1)$ form a weak Chebyshev system in $[-1, 1]$.

- Muntz System - Let $\eta_1 < \eta_2 < \cdots < \eta_m$. The family of functions $\{x^{\eta_1}, \ldots, x^{\eta_m}\}$ is a Chebyshev system on $(0, +\infty)$

- Let $\eta_1 < \eta_2 < \cdots < \eta_m$. The system of functions $e^{\eta_1}, xe^{\eta_1}, \ldots, e^{\eta_m}, xe^{\eta_m}$ is a Chebyshev system on $(0, +\infty)$.

- Trigonometric or Riesz interpolation - The family of functions $\{1, cosx, sinx, cos2x, sin2x, \ldots, cosmx, sinmx\}$ is a Chebyshev system in $[0, 2\pi)$

- The set of functions $\{1, cosx, cos2x, \ldots, cosmx\}$ is a Chebyshev system on $[0, \pi)$ and also $\{sinx, sin2x, \ldots, sinmx\}$ in $(0, \pi)$.

- With concentrated singularities- The family of functions: $\{1, \psi(x), x, x\psi(x), \ldots, x^{l-1}\psi(x), x^l\}$ where $\psi(x) = log(x + \delta)$ or $\psi(x) = (x + \delta)^\alpha$, with $\alpha > -1$ are Chebyshev systems.

4.2 Stability of interpolation on Gauss nodes

A remark on interpolation on Gauss nodes for Chebyshev orthonormal systems

As seen, if $\{\phi_i(x)\}_{i=1,\ldots,m}$ is a Chebyshev system then there exists a unique solution to the interpolation problem: $\underline{a} = B^{-1}\underline{f}$ where $B = (b_{ji}), b_{ji} = \phi_i(x_j)$. Let us see something on it's condition number. Suppose now that the functions $\{\phi_i(x)\}$ are orthonormal w.r.t. $d\mu$ and that the quadrature rue respects this orthogonality property:

$$\int \phi_i(x)\phi_j(x)\, d\mu = \delta_{ij}\,,\ \sum_{p=1}^{n} w_p \phi_i(x_p)\phi_j(x_p) = \delta_{ij}$$

In this hypothesis the matrix $A = (a_{ij})\,,\ a_{ij} = \sqrt{w_j}\phi_i(x_j)$ is orthogonal. thus we have $B^{-1} = A * D$ where D is the diagonal matrix $d_{ii} = \sqrt{w_i}$

In this case we can say: whenever the nodes of a generalized Gaussian quadrature formula are used as interpolation nodes, the resulting interpolation formula tends to be stable.

This is because, as long as the quadrature formula is reasonably accurate for all pairwise products of the functions $\phi_i(x)$, the matrix A is close to being orthogonal; therefore, the condition number of A is close to unity, and the interpolation based on the nodes $\xi_1, \xi_2, \ldots, \xi_n$ is stable.

4.3 Hermite Systems

A particular case of Chebyshev systems are the so called extended Chebyshev systems for which the determinant condition is required also for some of the derivatives of the functions.

Let us see in particular the case that leads to uniqueness of Hermite interpolation. We will say that a family of functions $\{\phi_i(x)\}_{i=1,\ldots,2n}$ is an extended Hermite system if $\phi_i \in C^1$, $\{\phi_i(x)\}$ is a Chebyshev system and the matrix F defined as:

$$F = \begin{pmatrix} \phi_1(x_1) & \phi_2(x_1) & \ldots & \phi_{2n}(x_1) \\ \phi_1(x_2) & \phi_2(x_2) & \ldots & \phi_{2n}(x_2) \\ \vdots & \vdots & & \vdots \\ \phi_1(x_n) & \phi_2(x_n) & \ldots & \phi_{2n}(x_n) \\ \phi_1'(x_1) & \phi_2'(x_1) & \ldots & \phi_{2n}'(x_1) \\ \vdots & \vdots & & \vdots \\ \phi_1'(x_n) & \phi_2'(x_n) & \ldots & \phi_{2n}'(x_n) \end{pmatrix}$$

is such that $det(F) \neq 0 \; \forall x_j \; s.t., \; j = 1, \ldots, n \; a \leq x_1 < x_2 < \cdots < x_n \leq b$.

It turns out that the columns of the inverse of the matrix F are exactly the vectors α_i and β_i that solve the Hermite interpolation problem:

- given the set of nodes $\{x_i\}$
- find α_{ih} and β_{ih} such that: $\sigma_i(x) = \sum_h \alpha_{ih}\phi_h(x)$, $\eta_i(x) = \sum_h \beta_{ih}\phi_h(x)$ and:

$$\begin{cases} \sigma_i(x_j) & = & 0 \\ \sigma_i'(x_j) & = & \delta_{ij} \end{cases} \begin{cases} \eta_i(x_j) & = & \delta_{ij} \\ \eta_i'(x_j) & = & 0 \end{cases} .$$

(Thus invertibility of the matrix F coincides to the existence and uniqueness of the solution to the Hermite interpolation problem)

Examples are:

- Polynomials
- Muntz System - Let $\eta_1 < \eta_2 < \cdots < \eta_m$. The set of functions $\{x^{\eta_1}, \ldots, x^{\eta_m}\}$ is a Hermite system on $(0, +\infty)$
- The exponentials $\{e^{\lambda_1 x}, e^{\lambda_1 x}, \ldots, e^{\lambda_n x}\}$ form an Hermite system for any $\lambda_1, \ldots, \lambda_n > 0$ on the interval $[0, 1)$.

5 Construction of the formulae

For the construction of generalized Gauss quadrature formulae the proposed algorithms take in account the resolution of one of the two nonlinear systems (each of the two define the quadrature rule uniquely): $\underline{\mathcal{F}} = \underline{0}$; $\underline{\mathcal{G}} = \underline{0}$.

$$\mathcal{F}_i(x_1, \dots, x_n) = \int \sigma_i(x)\, d\mu \quad i = 1, \dots, n$$

$$\mathcal{G}_j(x_1, \dots, x_n, w_1, \dots, w_n) = \left[\sum_{i=1}^{n} w_i \phi_j(x_i) \right] - M_j \quad j = 1, \dots, 2n$$

For both this functionals the Jacobian can be calculated explicitly, and thus Newton algorithm can be implemented.

In the case of functional $\underline{\mathcal{F}}$ the explicit calculation of the Jacobian and an elegant result on quadratic convergence of Newton's algorithm with inexact Jacobian can be found in Theorem 4.5 of:

Reference
J. Ma, V. Rokhlin, and S.Wandzura, Generalized Gaussian quadrature rules for systems of arbitrary functions, SIAM J. Numer. Anal. 33 (1996), no. 3, 971–996.

The case of functional $\underline{\mathcal{G}}$ is considered in the two works:

References
N. Yarvin and V. Rokhlin ”Generalized Gaussian quadratures and singular value decomposition of integral operators”, SIAM J. SCI. COMPUT. Vol. 20 (1998), No. 2, pp. 699–718; H. Cheng, N. Yarvin and V. Rokhlin ”Nonlinear optimization, quadrature and interpolation”, SIAM J. OPTIM. Vol. 9 (1999), No. 4, pp. 901–923

In this case the Jacobian is exactly the matrix $J = D{*}F$ where $D = diag(1, dots, 1, w_1, \dots, w_n,$ and also in this case the (local) quadratic convergence can be proven.

Drawback of all this procedure is the ill condition of the numerical problem that imposes to:

- Find a starting pont for Newton algorithm in a proper manner (continuation algorithm)
- Eventually modify the functions $\phi_i(x)$ in order to obtain better stability (projection and orthogonalization)