n-weight Gauss Quadrature for Quasi Definite Linear Functionals

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Introduction

Measure and Quadrature

Let μ be a non-decreasing distribution function defined on the real axis such that

$$\int_{\mathbb{R}} x^i \, d\mu(x) = m_i < \infty \text{ for all } i = 0, 1, 2, \ldots .$$

the moments of every order are finite

Given a real function f we are interested in the approximation of a Riemann-Stieltjes integral obtained by quadrature rules, that is

$$\int_{\mathbb{R}} f(x)\, d\mu(x) \approx \sum_{j=1}^{n} f(\lambda_j)\, \omega_j,$$

given certain nodes λ_j and weights ω_j.

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given certain nodes λ_j and weights ω_j.

If for every polynomial p of degree $\leq 2n-1$

$$\int_{\mathbb{R}} p(t)\, d\mu(t) = \sum_{j=1}^{n} p(\lambda_j)\, \omega_j,$$

then the rule is called Gauss quadrature rule.

Gauss quadrature properies

- G1: The n-node Gauss quadrature attains the maximum possible algebraic degree of exactness which is $2n - 1$.
- G2: If n-node Gauss quadrature exists it is unique, and j-node Gauss quadratures for $j = 1, \dots, n-1$ exist and are unique.
- G3: The Gauss quadrature can be written in the form $\mathbf{e}_1^T f(J_n)\,\mathbf{e}_1$, where J_n is a real symmetric tridiagonal matrix determined by the first $2n$ moments of the integral.

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Our goal is to give a formula with the same properties, for the approximation of a class of linear functionals.

Linear Functionals

Let $\mathcal{L}$ be a *linear* functional on the space of (complex) polynomials,

$$\mathcal{L} : \mathcal{P} \to \mathbb{C}.$$

$\mathcal{L}$ has finite complex moments

$$\mathcal{L}(x^k) = m_k, \quad k = 0, 1, \dots .$$

m_k is the moment of order k of the functional.

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Orthogonal Polynomials

We say that a sequence of polynomials $\{p_j\}_{j=0}^{\infty}$ is a sequence of *orthogonal polynomials with respect to the linear functional* $\mathcal{L}$ if:

1. $\deg(p_j) = j$ (p_j is of degree j),
2. $\mathcal{L}(p_i\, p_j) = 0$, for $i \neq j$,
3. $\mathcal{L}(p_j^2) \neq 0$.

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Existence of Orthogonal Polynomials

Hankel determinants

$$\Delta_j = \begin{vmatrix} m_0 & m_1 & \dots & m_j \\ m_1 & m_2 & \dots & m_{j+1} \\ \vdots & \vdots & \ddots & \vdots \\ m_j & m_{j+1} & \dots & m_{2j} \end{vmatrix} .$$

Quasi-definite linear functional

A linear functional $\mathcal{L}$ for which the first k Hankel determinants are nonzero, i.e. $\Delta_j \neq 0$ for $j = 0, 1, \dots, k$, is called quasi-definite on $\mathcal{P}_k$ the space of polynomials of degree at most k.

There exists a (unique up to nonzero multiplicative factors) sequence $\{p_j\}_{j=0}^{k}$ of orthogonal polynomials with respect to $\mathcal{L}$ if and only if $\mathcal{L}$ is quasi-definite on $\mathcal{P}_k$.

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Positive definite functionals

Positive definite linear functional

The linear functional $\mathcal{L}$ is said to be positive definite on $\mathcal{P}_k$ if $\Delta_j > 0$ and $m_j \in \mathbb{R}$, for $j = 0, \ldots, k$.

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Three-term recurrence relation

If $p_0, p_1, \ldots, p_n$ exist, then for $k = 1, 2, \ldots, n$,

$$\beta_k p_k(x) = (x - \alpha_{k-1}) p_{k-1}(x) - \gamma_{k-1} p_{k-2}(x),$$

with $p_{-1}(x) = 0$, $p_0(x) = c \neq 0$ given and $\alpha_{k-1}, \beta_k, \gamma_{k-1}$ nonzero scalars.

$$T_n = \begin{pmatrix} \alpha_0 & \gamma_1 & & & \\ \beta_1 & \alpha_1 & \gamma_2 & & \\ & \ddots & \ddots & \ddots & \\ & & \beta_{n-2} & \alpha_{n-2} & \gamma_{n-1} \\ & & & \beta_{n-1} & \alpha_{n-1} \end{pmatrix} \qquad \mathbf{p} = \begin{pmatrix} p_0(\xi) \\ p_1(\xi) \\ \vdots \\ p_{n-2}(\xi) \\ p_{n-1}(\xi) \end{pmatrix}$$

$$\xi \mathbf{p} = T_n \, \mathbf{p} + \gamma_n p_n(\xi) \, \mathbf{e_n}$$

Theorem: the eigenvalues of T_n are the zeros of p_n.

Remark 1: The matrix T_n is fully determined by the orthogonal polynomials $p_0, \dots, p_{n-1}$ and by the moments $m_0, \dots, m_{2n-1}$.

Remark 2: If we rescale the orthogonal family $p_0, \dots, p_{n-1}$ we obtained a different tridiagonal matrix $\overline{T}_n$.

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Jacobi matrices

We say an Orthonormal family of polynomials an orthogonal family of polynomials such that

$$\mathcal{L}(p_i^2) = 1.$$

The tridiagonal matrix associated with this family is symmetric.

Jacobi matrix

A square complex matrix is called *Jacobi matrix* if it is tridiagonal, symmetric and has no zero elements on its sub- and super-diagonal.

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Moments Matching Property

an extension

We proved the following theorem

Theorem

Let $\mathcal{L}$ be a quasi-definite linear functional on $\mathcal{P}_n$ and let J_n be a Jacobi matrix determined by the firs $2n$ moments of $\mathcal{L}$. Then we have that

$$\mathcal{L}(x^i) = \mathbf{e}_1^T (J_n)^i \, \mathbf{e}_1, \quad i = 0, \dots, 2n-1. \tag{1}$$

Remark: In the case of positive definite linear functional this property is well known and it is part of the classical theory on the Gauss quadrature.
Moreover, it was proved also in the case of discrete linear functional

$$\mathcal{L}(f) = \mathbf{u}^* f(A) \, \mathbf{v}$$

(see Strakoš [5])

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n-weight Gauss Quadrature

Positive definite case (classical)

We recall that in the classical theory ($\mathcal{L}$ positive definite) we get

$$\mathcal{L}(f) = \int_{\mathbb{R}} f(t) \mathrm{d}\,\mu(t) = \mathbf{e}_1^T f(J_n) \mathbf{e}_1 = \sum_{i=1}^{n} \omega_i f(\lambda_i)$$

for $deg(f) \leq 2n - 1$.

- J_n is real, hence it is Hermitian and has n distinct eigenvalues (diagonalizable)
- J_n can be compute by the (Hermitian) Lanczos algorithm for $\mathcal{L}$ discrete
- the nodes λ_i are the eigenvalues of J_n
- (every weight ω_i can be obtained by the eigenvector associated with λ_i)

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Diagonalizable case

Now, let $\mathcal{L}$ quasi definite on $\mathcal{P}_n$ and let J_n diagonalizable. Then we can easily extend the classical Gauss Quadrature (see Saylor and Smolarski [4]).

$$\mathcal{L}(f) = \mathbf{e}_1^T f(J_n)\mathbf{e}_1 = \sum_{i=1}^{n} \omega_i f(\lambda_i)$$

for $deg(f) \leq 2n - 1$.
The nodes λ_i are the n complex eigenvalues of J_n.

Diagonalizable case

The quadrature rule have the properties G1 and G2 if and only if:

1. $\mathcal{L}$ is quasi-definite on $\mathcal{P}_n$
2. J_n is diagonalizable

Or equivalently

1. There exists a sequence of orthogonal polynomials $p_0, \ldots, p_n$ with respect to $\mathcal{L}$
2. Zeros of p_j, $j = 1, \ldots, n$, are distinct.

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Complex Jacobi matrices

Remark: J_n is Hermitian $\Leftrightarrow$ it is real.

A complex Jacobi matrix may not always be diagonalizable

What happen when J_n is not diagonalizable?

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Complex tridiagonal matrices

Theorem (Wilkinson [7])

Every tridiagonal matrix $T \in \mathbb{C}^{n \times n}$ with nonzero elements on its super-diagonal (and sub-diagonal) is non-derogatory, i.e. each one of its eigenvalues has geometric multiplicity 1.

Corollary

Every complex tridiagonal matrix without any zero entry on super-diagonal (and sub-diagonal) is diagonalizable if and only if it has distinct eigenvalues.

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Non-derogatory matrices

If a matrix is non-derogatory

- every eigenvalue λ has geometric multiplicity 1.
- That means that the eigenspace of λ has dimension 1
- Hence, there exists only one eigenvector for λ.
- Moreover, there exist only one Jordan block corresponding to λ.

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G1, G2 and G3 properties

However, the moments matching property still holds both for J_n diagonalizable or nondiagonalizable.

If we want a quadrature rule satisfying G1 and G2 whenever $\mathcal{L}$ is quasi-definite, we have to define a quadrature in the form

n-weight quadrature rule (P., Pranić, Strakoš, submitted)

$$\mathcal{L}(f) = \sum_{i=1}^{\ell} \sum_{j=0}^{s_i-1} \omega_{i,j} \, f^{(j)}(\lambda_i) + R_n(f),$$

where $s_1 + \cdots + s_\ell = n$.

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Algebraic exactness

Theorem (P., Pranić, Strakoš, submitted)

The n-weight quadrature is exact for every f from $\mathcal{P}_{2n-1}$ if and only if it is exact on $\mathcal{P}_{n-1}$ and the polynomial

$$\varphi_n(x) = (x-\lambda_1)^{s_1}(x-\lambda_2)^{s_2}\dots(x-\lambda_\ell)^{s_\ell}$$

satisfies $\mathcal{L}(\varphi_n\, p) = 0$ for every $p \in \mathcal{P}_{n-1}$.

G1 and G2 hold if and only if

- $\varphi_0, \dots, \varphi_n$ are orthogonal polynomials ($\mathcal{L}$ is quasi-definite on $\mathcal{P}_n$);
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Hence, for the existence of the formula we only need $\Delta_{n-1} \neq 0$ while, to have degree of exactness $2n-1$ we need $\Delta_n \neq 0$. Otherwise, we can have a grater degree of exactness.

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Example

Let linear functional $\mathcal{L}$ defined by the sequence of moments

$$1, 3, 8, 20, 52, 156, i, \dots,$$

The 2-node quadrature of degree of exactness 3 does not exist since the zeros of π_2 are $x_1 = x_2 = 2$.
We can use 2-weight quadrature of the form $\omega_{1,1} f(2) + \omega_{1,2} f'(2)$.

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Let linear functional $\mathcal{L}$ defined by the sequence of moments

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Example

Notice that its degree of exactness would be higher if and only if

$$m_4 = 2^4 + 4 \cdot 2^3 = 48.$$

In this case we would have $\Delta_2 = 0$, i.e. $\mathcal{L}$ would not be quasi-definite on $\mathcal{P}_2$. If

$$m_5 = 2^5 + 5 \cdot 2^4 = 112$$

then the quadrature $f(2) + f'(2)$ would have degree of exactness at least 5. And so on...
We cannot determined the degree of exactness of the formula just knowing m_1, m_2, m_3.

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Summarizing, the n-weight quadrature formula

$$\sum_{i=1}^{\ell} \sum_{j=0}^{s_i-1} \omega_{i,j} \, f^{(j)}(\lambda_i)$$

satisfies G1, G2 and G3 if and only if $\mathcal{L}$ is quasi-definite on $\mathcal{P}_n$. That is why we think that such a quadrature should be referred to as n-weight Gauss quadrature.

Moreover,

- J_n can be compute by the (non-Hermitian) Lanczos algorithm for $\mathcal{L}$ discrete
- the nodes λ_i are the eigenvalues of J_n with algebraic multiplicity s_i
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Gauss quadrature for quasi-definite linear functionals,
submitted.

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Thank you for your attention!