Numerical analysis: Gaussian quadrature

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1 Orthogonal systems

Definition 1. V vector space over a field $\mathbb{F} \subseteq \mathbb{C}$, $u, v \in V$. **An inner product** is a function $\langle u, v\rangle \in \mathbb{F}$ s.t.

1. $\langle u, u\rangle \geq 0$, and $\langle u, u\rangle = 0$ iff $u = 0$;
2. $\langle v, u\rangle = \overline{\langle u, v\rangle}$ ($\overline{x}$ denotes the complex conjugate)
3. $\langle u_1 + u_2, g\rangle = \langle u_1, g\rangle + \langle u_2, g\rangle$
4. $\langle \alpha u, v\rangle = \alpha \langle u, v\rangle$

Definition 2. Let f, g be continuous in $[a, b]$ and $w(x) \geq 0$ continuous in (a, b) possibly with a finite number of zeros. Let

$$\langle f, g\rangle_w = (f, g)_w = \langle f, g\rangle = (f, g) = \int_a^b f(x)\, g(x)\, w(x)\, dx. \tag{1}$$

This is an inner product in the space $V = C[a, b]$ of continuous functions in $[a, b]$, over the field $\mathbb{F} = \mathbb{R}$. f, g are **orthogonal** if $\langle f, g\rangle = 0$. We also write $f \perp g$.

Definition 3. The system of **orthogonal polynomials** w.r.t an inner product is the set of polynomials $Q_0 \in \Pi_0, \dots, Q_n \in \Pi_n, \dots$, s.t. $Q_i \perp Q_j$ for all $i \neq j$.

Claim 1. $Q_k \perp \Pi_{k-1}$ for $k = 1, \dots, n$.

There always exists a system of orthogonal polynomials wrt. the inner product (1).

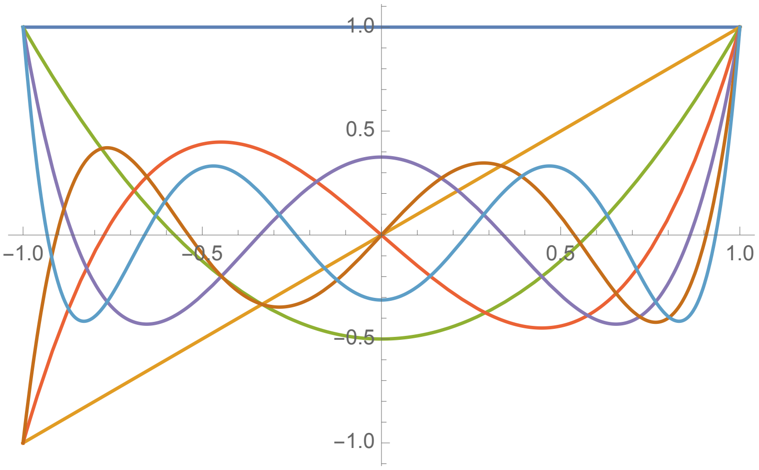

Figure 1: First Legendre polynomials

Proof. Can be shown by performing Gram-Schmidt orthogonalization procedure starting with the monomials $\{1, x, x^2, \ldots, x^n, \ldots\}$. In such a way the OP are unique up to a constant. $\square$

Example 1 (Legendre polynomials)**.** $w(x) = 1$ on the interval $[-1, 1]$. The OP obtained are called **Legendre polynomials.** Without proof, we present the following facts:

$$P_n(x) = \frac{(-1)^n}{2^n n!}\frac{d^n}{dx^n}\left[\left(1-x^2\right)^n\right], \quad n = 0, 1, 2, \ldots \quad \text{Rodrigues' formula}$$

$$P_{n+1}(x) = \frac{2n+1}{n+1}xP_n(x) - \frac{n}{n+1}P_{n-1}(x), \quad n = 1, 2, \ldots \quad \text{Recursion formula}$$

$$P_0(x) = 1 \quad , \quad P_1(x) = x, \quad P_2(x) = \frac{1}{2}\left[3x^2 - 1\right]$$

Example 2 (Chebyshev polynomials)**.** $w(x) = \frac{1}{\sqrt{1-x^2}}$ on $(-1, 1)$:

$$T_n(x) = \cos n(\arccos x), \quad n = 0, 1, 2, \ldots$$
$$T_0(x) = 1, \quad T_1(x) = x, \quad T_2(x) = 2x^2 - 1$$

Properties:

1. Recursion:

$$T_{n+1}(x) = 2xT_n(x) - T_{n-1}(x), \quad n = 1, 2, \ldots$$
$$T_0(x) = 1 \quad , \quad T_1(x) = x$$

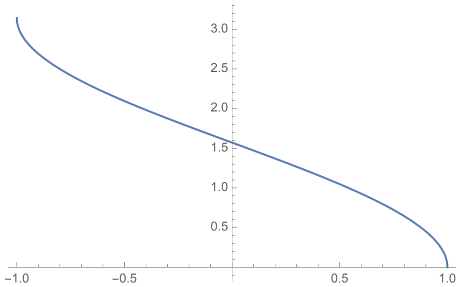

Figure 2: $y = \arccos x$

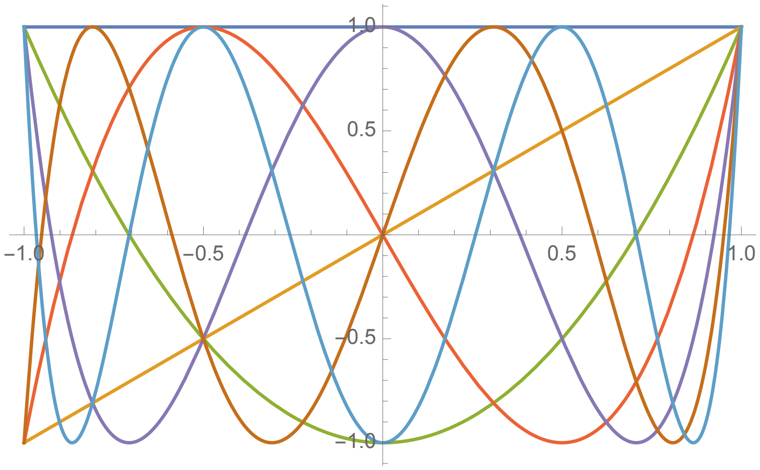

Figure 3: First Chebyshev polynomials

This can be shown using the identity $\cos\alpha + \cos\beta = 2\cos\left(\frac{\alpha+\beta}{2}\right)\cos\left(\frac{\alpha-\beta}{2}\right)$:

$$\begin{aligned} T_{n+1}(x)+T_{n-1}(x) &= \cos\underbrace{((n+1)\arccos x)}_{\alpha} + \cos\underbrace{((n-1)\arccos x)}_{\beta} \\ &= 2\cos\underbrace{(n\arccos x)}_{(\alpha+\beta)/2}\cos\underbrace{(\arccos(x))}_{(\alpha-\beta)/2} = 2xT_n(x), \quad n = 1, 2, \dots \end{aligned}$$

Therefore $T_n(x)$ is a polynomial of degree n.

2. Orthogonality:

$$\begin{aligned} \langle T_n(x), T_m(x)\rangle &= \int_{-1}^{1} \frac{\cos(n\cdot\arccos x)\cos(m\cdot\arccos x)}{\sqrt{1-x^2}}dx \\ \left[x = \cos\theta, \theta = \arccos x, \theta' = -\left(1-x^2\right)^{-1/2}\right] &= -\int_{\pi}^{0} \cos(n\cdot\theta)\cos(m\cdot\theta)d\theta \\ &= \int_0^{\pi} \cos(n\cdot\theta)\cos(m\cdot\theta)d\theta \\ [m \neq n] &= \frac{1}{2}\int_0^{\pi} (\cos(n-m)\theta + \cos(n+m)\theta)d\theta = 0 \end{aligned}$$

3. The leading coefficient of $T_n(x)$ is 2^{n-1}.

4. $T_n(x)$ has n (simple) roots in $(-1, 1)$: $x_k = x_{k,n} = \cos\left[\frac{2k+1}{n}\cdot\frac{\pi}{2}\right]$ for $k = 0, \dots, n-1$:

$$T_n(x_{k,n}) = \cos n\left[\frac{2k+1}{n}\cdot\frac{\pi}{2}\right] = \cos\left[(2k+1)\frac{\pi}{2}\right] = 0.$$

5. $|T_n(x)| \le 1$ in $[-1, 1]$ with $n+1$ extremal points $v_k = v_{k,n} = \cos\left[\frac{k\pi}{n}\right], \quad k = 0, 1, \dots n$. Indeed:

$$T_n(v_{k,n}) = \cos n\left[\frac{k\pi}{n}\right] = \cos[k\pi] = (-1)^k.$$

Example 3 (Laguerre polynomials)**.** $w(x) = e^{-x}$ on the semi-infinite interval $[0, \infty)$. Recursion formula:

$$\begin{array}{l} L_{n+1}(x) = \left(\frac{2n+1}{n+1} - \frac{x}{n+1}\right)L_n(x) - \frac{n}{n+1}L_{n-1}(x), \quad n = 1, 2, \dots \\ L_0(x) = 1 \quad , \quad L_1(x) = 1 - x \end{array}.$$

Example 4 (Hermite polynomials)**.** $w(x) = e^{-x^2}$ on the interval $(-\infty, +\infty)$. Recursion formula:

$$\begin{array}{l} H_{n+1}(x) = 2xH_n(x) - 2nH_{n-1}(x), \quad n = 1, 2, \dots \\ H_0(x) = 1, \quad H_1(x) = 2x. \end{array}$$

2 Gaussian quadrature rules

Fixing a weight $w(x)$, we look for an integration rule of the form

$$I(f)=\int_a^b f(x)\omega(x)dx \approx \sum_{i=0}^{n} A_i f(x_i)=\tilde{I}(f). \tag{2}$$

We will look to determine $\{A_i,x_i\}_{i=0}^n$, overall $2n+2$ parameters. The rule will be exact for polynomials $P\in\Pi_{2n+1}$.

Theorem 1. *If $\{x_i\}_{i=0}^n$ are the roots of Q_{n+1}, the orthogonal polynomial of degree $n+1$ with respect to the inner product (1), and the coefficients $\{A_i\}_{i=0}^n$ are determined by the formulas*

$$A_i=\int_a^b \ell_i(x)\omega(x)dx, \quad i=0,\dots,n, \tag{3}$$

then the formula (2) is exact for polynomials of degree at most $2n+1$, with the error

$$E(I(f))=I(f)-\tilde{I}(f)=\int_a^b f[x_0,x_1,\dots,x_n,x_0,x_1,\dots,x_n,x]\ \underbrace{q_{n+1}^2(x)}_{\prod_{k=0}^n (x-x_k)^2}\ \omega(x)dx=$$

$$=\frac{f^{(2n+2)}(\xi)}{(2n+2)!}\int_a^b q_{n+1}^2(x)\,\omega(x)dx.$$

2.1 First proof

Consider the interpolation polynomial P_n to $f(x)$ at the nodes $a\le x_0<x_1<\cdots<x_n\le b$. We know that

$$I(f)=\underbrace{\int_a^b P_n(x)w(x)\,dx}_{\tilde{I}(f)}+\underbrace{\int_a^b f[x_0,x_1,\dots,x_n,x]\,q_{n+1}(x)\,w(x)\,dx}_{E(I(f))}.$$

Clearly we have $q_{n+1}(x)=\alpha_n Q_{n+1}(x)$. By Claim 1 we have $\langle Q_{n+1},1\rangle=\int_a^b Q_{n+1}(x)\,w(x)\,dx=0$. Therefore $\langle q_{n+1},1\rangle=0$ as well. As in the development of **Case B** in the previous lecture, we have for every x_{n+1}

$$\begin{aligned}
f[x_0,x_1,\dots,x_n,x_{n+1},x]&=\frac{f[x_0,x_1,\dots,x_n,x]-f[x_0,x_1,\dots,x_n,x_{n+1}]}{x-x_{n+1}}\\
f[x_0,x_1,\dots,x_n,x]&=f[x_0,x_1,\dots,x_n,x_{n+1}]+f[x_0,x_1,\dots,x_n,x_{n+1},x](x-x_{n+1})\\
E(I(f))&=\int_a^b f[x_0,x_1,\dots,x_n,x]\,q_{n+1}(x)\,w(x)\,dx\\
&=\int_a^b \{f[x_0,x_1,\dots,x_n,x_{n+1}]+f[x_0,x_1,\dots,x_n,x_{n+1},x](x-x_{n+1})\}\,q_{n+1}(x)\,w(x)\,dx\\
&=\int_a^b f[x_0,x_1,\dots,x_n,x_{n+1},x](x-x_{n+1})\,q_{n+1}(x)\,w(x)\,dx.
\end{aligned}$$

Put $r_{n+2}(x) = (x - x_{n+1}) q_{n+1}(x)$. We have $\int_a^b r_{n+2}(x) w(x)\, dx = \langle q_{n+1}, x - x_{n+1} \rangle = 0$ (since $Q_{n+1} \perp \Pi_1$). Therefore we can apply the computation again, and get that for every x_{n+2}

$$\begin{aligned} E(I(f)) &= \int_a^b f[x_0, x_1, \dots, x_n, x_{n+1}, x]\, r_{n+2}(x) w(x)\, dx \\ &= \int_a^b f[x_0, x_1, \dots, x_n, x_{n+1}, x_{n+2}, x]\, (x - x_{n+2}) r_{n+2}(x) w(x)\, dx. \end{aligned}$$

Again, $\langle r_{n+2}, x - x_{n+2} \rangle = \langle q_{n+1}, (x - x_{n+1})(x - x_{n+2}) \rangle = 0$ since $Q_{n+1} \perp \Pi_2$. Continuing in this fashion, we obtain that for every choice of $x_{n+1}, \dots, x_{2n+1}$ we have

$$E(I(f)) = \int_a^b f[x_0, x_1, \dots, x_n, x_{n+1}, x_{n+2}, \dots, x_{2n+1}, x]\, (x - x_{2n+1}) r_{2n+1}(x) w(x)\, dx$$

where $r_{2n+1}(x) = q_{n+1}(x)(x - x_{n+1}) \cdots (x - x_{2n})$.

Now we choose $x_{n+k+1} = x_k$ for $k = 0, \dots, n$. Therefore $(x - x_{2n+1}) r_{2n+1}(x) = q_{n+1}^2(x)$, and by Claim 1 from Lecture 5 and Claim 5 from Lectures 1-3 (which holds for repeated nodes as well) we conclude that

$$\begin{aligned} E(I(f)) &= \int_a^b f[x_0, x_1, \dots, x_n, x_0, x_1, \dots, x_n, x]\, q_{n+1}^2(x) w(x)\, dx \\ &= \frac{f^{(2n+2)}(\xi)}{(2n+2)!} \int_a^b q_{n+1}^2(x) \omega(x) dx, \end{aligned}$$

finishing the proof. □

2.2 Second proof

As in the first proof, consider the interpolation polynomial P_n to $f(x)$ at the nodes $a \le x_0 < x_1 < \cdots < x_n \le b$. Using Lagrange's form of P_n we obtain

$$\langle P_n, 1 \rangle = \int_a^b P_n(x)\omega(x) dx = \int_a^b \sum_{i=0}^n f(x_i)\, \ell_i(x)\omega(x) dx = \sum_{i=0}^n f(x_i) \underbrace{\int_a^b \ell_i(x)\omega(x) dx}_{A_i} = \sum_{i=0}^n A_i f(x_i).$$

Now consider the Hermite interpolation polynomial $P_{2n+1}(x)$ to f where each node is doubled, i.e. $\{x_0, x_0, \ldots, x_n, x_n\}$.

$$\begin{aligned}
e(x) &= P_{2n+1}(x) - P_n(x), \quad \deg e = 2n+1 \\
e(x_i) &= 0 \quad i = 0, 1, \ldots, n \\
\Longrightarrow e(x) &= q_{n+1}(x)\, s(x), \quad s(x) \in \Pi_n \\
\Longrightarrow \langle P_{2n+1}, 1\rangle &= \langle P_n, 1\rangle + \langle q_{n+1}s, 1\rangle \\
&= \sum_{i=0}^{n} A_i f(x_i) + \underbrace{\langle q_{n+1}, s\rangle}_{=0} \qquad [q_{n+1} \perp \Pi_n]
\end{aligned}$$

$$\langle P_{2n+1}, 1\rangle = \int_a^b P_{2n+1}(x)\omega(x)dx = \sum_{i=0}^{n} A_i f(x_i). \tag{4}$$

Now let $p(x) \in \Pi_{2n+1}$ be any polynomial, then it coincides with its Hermite interpolation polynomial P_{2n+1} at the nodes $\{x_0, x_0, \ldots, x_n, x_n\}$, and therefore (4) is exact for p.

By the formula (7) for Hermite interpolation error from Lectures 1-3, applied with $2n+2$ nodes as above, we have

$$f(x) = P_{2n+1}(x) + f[x_0, x_0, \ldots, x_n, x_n, x]\, \underbrace{q_{2n+2}(x)}_{=q_{n+1}^2(x)}.$$

Integrating and using the integral mean value theorem together with Claim 5 from Lectures 1-3, we get

$$\begin{aligned}
\int_a^b f(x)\, w(x)\, dx &= \int_a^b P_{2n+1}(x)\omega(x)dx + \int_a^b f[x_0, x_0, \ldots, x_n, x_n, x]\, q_{n+1}^2(x)\, w(x)\, dx \\
&= \sum_{i=0}^{n} A_i f(x_i) + \frac{f^{(2n+2)}(\xi)}{(2n+2)!} \int_a^b q_{n+1}^2(x)\, w(x) dx,
\end{aligned}$$

completing the proof. □

3 Examples

Example 5. Approximate $\int_{-1}^{1} f(x)dx \approx A_0 f(x_0)$ by using Gaussian quadrature.

Solution. Here $n = 0$, the formula should be exact for $f = 1, x$:

$$\int_{-1}^{1} 1dx = 2 = A_0$$

$$\int_{-1}^{1} xdx = 0 = A_0 x_0 \Rightarrow x_0 = 0$$

and so $\int_{-1}^{1} f(x)dx \approx 2f(0)$.

Alternatively, we can use the zero of the Legendre polynomial $P_1(x) = x$, i.e. $x_0 = 0$. To find A_0, we require exactness for Π_0, i.e. $f = 1$:

$$\int_{-1}^{1} 1dx = 2 = A_0,$$

as before.

To compute the error, set $q_1(x) = x$ and then

$$E(I(f)) = \frac{f''(c)}{2}\int_{-1}^{1} q_1^2(x)\,dx = \frac{f''(c)}{3}.$$

Example 6. Approximate $\int_{-1}^{1}\frac{f(x)}{\sqrt{1-x^2}}dx$ by Gaussian quadrature using interpolation polynomial of degree at most 2.

Solution. $n = 2$, we should use the Chebyshev polynomial $T_{n+1}(x) = T_3(x) = 4x^3 - 3x$ whose roots are $x_0 = -\frac{\sqrt{3}}{2}, x_1 = 0, x_2 = \frac{\sqrt{3}}{2}$.

To find the coefficients, we require (2) to be exact for $f = 1, x, x^2$:

$$\begin{aligned}
\pi &= \int_{-1}^{1}\frac{1}{\sqrt{1-x^2}}dx = A_0 + A_1 + A_2\\
0 &= \int_{-1}^{1}\frac{x}{\sqrt{1-x^2}}dx = (A_2 - A_0)\frac{\sqrt{3}}{2} \Longrightarrow A_0 = A_2\\
\frac{\pi}{2} &= \int_{-1}^{1}\frac{x^2}{\sqrt{1-x^2}}dx = \frac{3}{4}(A_0 + A_2) \Longrightarrow A_0 = A_2 = \frac{\pi}{3} \Longrightarrow A_1 = \frac{\pi}{3}.
\end{aligned}$$

Finally

$$\begin{aligned}
\int_{-1}^{1}\frac{f(x)}{\sqrt{1-x^2}}dx &\approx \frac{\pi}{3}\cdot f\left(-\frac{\sqrt{3}}{2}\right) + \frac{\pi}{3}\cdot f(0) + \frac{\pi}{3}\cdot f\left(\frac{\sqrt{3}}{2}\right)\\
E(I(f)) =&\frac{f^{(6)}(\xi)}{6!}\int_{-1}^{1}\frac{q_3^2(x)}{\sqrt{1-x^2}}dx = \frac{f^{(6)}(\xi)}{6!}\int_{-1}^{1}\frac{x^2\left(x^2-\frac{3}{4}\right)^2}{\sqrt{1-x^2}}dx.
\end{aligned}$$

Example 7. Approximate $\int_{-1}^{1} f(x)dx \approx A_0 f(x_0) + A_1 f(x_1)$ by using Gaussian quadrature.

Solution. $n = 1$ and we should use Legendre polynomial $P_{n+1}(x) = P_2(x) = \frac{1}{2}[3x^2 - 1]$, the roots are $\pm\frac{1}{\sqrt{3}}$. The linear system for the coefficients:

$$\begin{aligned}
2 &= \int_{-1}^{1} 1dx = A_0 + A_1\\
0 &= \int_{-1}^{1} xdx = (A_0 - A_1)\frac{1}{\sqrt{3}} \Longrightarrow A_0 = A_1 = 1.
\end{aligned}$$

The result is

$$\int_{-1}^{1} f(x)\,dx \approx f\left(-\frac{1}{\sqrt{3}}\right) + f\left(\frac{1}{\sqrt{3}}\right)$$

$$E(I(f)) = \frac{f^{(4)}(\xi)}{4!}\int_{-1}^{1} q_2^2(x)\,dx = \frac{f^{(4)}(\xi)}{4!}\int_{-1}^{1}\left(x^2-\frac{1}{3}\right)^2 dx = \frac{1}{135}f^{(4)}(\xi).$$

Example 8. Answer the following questions.

1. Compute the first 3 orthogonal polynomials with respect to the inner product

$$\langle f, g\rangle = \int_{-1}^{1} f(x)g(x)\left(1+x^2\right)dx.$$

2. What are the two Gaussian quadrature nodes $\{x_0, x_1\}$ for $n = 1$?
3. Approximate $\int_{-1}^{1} f(x)\left(1+x^2\right)dx$ using $\{x_0, x_1\}$ from 2).
4. Compute the error formula.

Solution. $w(x) = (1+x^2)$.

1. Let's use Gram-Schmidt on $\{f_0, f_1, f_2\} = \{1, x, x^2\}$:

$$\begin{aligned}
Q_0 &= f_0 = 1 \\
Q_1 &= f_1 - \frac{\langle f_1, Q_0\rangle}{\langle Q_0, Q_0\rangle}Q_0 = x - \langle x, 1\rangle \\
&= x - \frac{\underbrace{\int_{-1}^{1}\left(x+x^3\right)dx}_{=0}}{\underbrace{\int_{-1}^{1}\left(1+x^2\right)dx}_{=2+\frac{2}{3}=\frac{8}{3}}} = x \\
Q_2 &= x^2 - \frac{\overbrace{\left\langle x^2, 1\right\rangle}_{=\frac{2}{3}+\frac{2}{5}=\frac{16}{15}}}{\frac{8}{3}} - \frac{\overbrace{\left\langle x^2, x\right\rangle}_{=0}}{\langle x, x\rangle}x \\
&= x^2 - \frac{2}{5}.
\end{aligned}$$

2. The zeros of Q_2 are $\pm\sqrt{\frac{2}{5}}$.

3. The linear system for the coefficients A_0, A_1:

$$\frac{8}{3} = \int_{-1}^{1} \left(1 + x^2\right) dx = A_0 + A_1$$
$$0 = \int_{-1}^{1} x \left(1 + x^2\right) dx = \sqrt{\frac{2}{5}} \left(A_1 - A_0\right) \Longrightarrow A_0 = A_1 = \frac{4}{3}$$

and so

$$\int_{-1}^{1} f(x) \left(1 + x^2\right) dx \approx \frac{4}{3} \left\{ f\left(-\sqrt{\frac{2}{5}}\right) + f\left(\sqrt{\frac{2}{5}}\right) \right\}.$$

4. The error formula gives

$$E\left(I\left(f\right)\right) = \frac{f^{(4)}\left(c\right)}{24} \int_{-1}^{1} \left(1 + x^2\right) \left(x^2 - \frac{2}{5}\right) dx.$$