Numerical Calculus

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References

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Orthogonal functions (Burden *et al.*, 2022)

An integrable function w is called a *weight function* on $[a, b]$ if $w(x) \geqslant 0,\ \forall\, x \in [a, b]$ but $w \not\equiv 0$ on any subinterval of $[a, b]$.
$\phi_0, \ldots, \phi_n$ is said to be *linearly independent* on $[a, b]$ if, whenever

$$c_0\phi_0(x) + c_1\phi_1(x) + \ldots + c_n\phi_n(x) = 0, \quad \forall\, x \in [a, b]$$

we have $c_0 = c_1 = \ldots = c_n = 0$. Otherwise, the set of functions is said to be *linearly dependent.*
A finite or infinite sequence of functions $\phi_0, \ldots, \phi_n, \ldots$ constitutes an *orthogonal system* for the interval $[a, b]$ with respect to w if

$$\langle \phi_k, \phi_j \rangle_w = \int_a^b w(x)\phi_k(x)\phi_j(x)\, dx = \begin{cases} 0,\ j \neq k \\ \alpha_j > 0, j = k \end{cases} .$$

If, in addition, $\alpha_j = 1$ then the sequence is said to be *orthonormal*.

Orthogonal Polynomials (Dahlquist and Björk, 2008)

By a family of orthogonal polynomials we mean a triangle family of polynomials which (in the continuous case) is an orthogonal system with respect to a given inner product. The theory of orthogonal polynomials is also of fundamental importance for many problems which at first sight seem to have little connection with approximation (*e.g.*, numerical integration, continued fractions, and the algebraic eigenvalue problem).
The weight function w determines the orthogonal polynomials R_n up to a constant factor in each polynomial.

Orthogonal Polynomials (Dahlquist and Björk, 2008)

The orthogonal polynomials satisfy a number of relationships of the same general form. In the case of a continuously differentiable weight function w we have an explicit expression, *Rodrigue's formula*

$$R_n(x) = \frac{1}{a_n w(x)} \frac{d^n}{dx^n}\big(w(x)(g(x))^n\big), \; n = 0, 1, \dots$$

where g is a polynomial in x independent of n.
The orthogonal polynomials also satisfy a second order differential equation,

$$g_2(x)R_n''(x) + g_1(x)R_n'(x) + \lambda R_n(x) = 0$$

where g_1 and g_2 are independent of n and λ is a constant only dependent on n.

Orthogonal Polynomials (Quarteroni *et al.*, 2000)

For every weight function in an inner product space there is a triangle family of orthogonal polynomials R_n, $n = 0, 1, 2, \ldots$ such that R_n has exact degree n, and is orthogonal to all polynomials of degree less than n. The family is uniquely determined apart from the fact that the leading coefficients can be given arbitrary positive values. The monic orthogonal polynomials satisfy the *three-term recurrence formula*

$$\begin{cases} R_{n+1}(x) = (x - \alpha_n) R_n(x) - \beta_n R_{n-1}(x), \; n \geqslant 0 \\ R_{-1}(x) = 0, \quad R_0(x) = 1 \end{cases}$$

where

$$\alpha_n = \frac{\langle x R_n, R_n \rangle_w}{\langle R_n, R_n \rangle_w} \text{ and } \beta_{n+1} = \frac{\langle R_{n+1}, R_{n+1} \rangle_w}{\langle R_n, R_n \rangle_w}$$

The coefficient β_0 is arbitrary and is chosen according to the particular family of orthogonal polynomials at hand.

Orthogonal Polynomials (Doman, 2016)

We assume that the weight function $w(x) \geqslant 0$, $\forall\, x \in (a, b)$ is s.t. the *moments*

$$\mu_k = \int_a^b x^k w(x)\, dx$$

are defined for all $k \geqslant 0$ and $\mu_0 > 0$. We consider the set of orthogonal polynomials $R_0, R_1, \ldots$ with $\deg(R_k) = k$ and

$$\langle R_n, R_m \rangle_w = \int_a^b w(x) R_n(x) R_m(x)\, dx = 0, \text{ for } m \neq n.$$

It is clear that

$$h_n := \langle R_n, R_n \rangle_w = \int_a^b w(x) \big(R_n(x)\big)^2\, dx \geqslant 0.$$

Orthogonalisation Procedure (Doman, 2016)

For a given weight function w, this is an inductive procedure to generate a set of orthogonal polynomials starting from the zeroth order polynomial $R_0(x) = 1$. The procedure works by using the orthogonality condition to determine the coefficients of the powers of x in the polynomial $R_{n+1}(x)$ using all of the previously determined $R_m(x)$, $0 \leqslant m \leqslant n$.

The procedure consists of the following steps:

I. Set $R_0(x) = 1$

II. Set $R_1(x) = x + a_{1,0}$. The constant $a_{1,0}$ is determined by the orthogonality condition $R_1 \perp R_0$

$$\langle R_1, R_0 \rangle_w = \int_a^b w(x)(x + a_{1,0})\, dx = 0 \Leftrightarrow a_{1,0} = \frac{\displaystyle\int_a^b xw(x)\, dx}{\displaystyle\int_a^b w(x)\, dx}$$

Orthogonalisation Procedure (Doman, 2016)

The procedure consists of the following steps:

III. Set $R_2(x) = x^2 + a_{2,1}x + a_{2,0}$. The constants $a_{2,0}$ and $a_{2,1}$ are determined by orthogonality conditions $R_2 \perp R_0$, $R_2 \perp R_1$

$$\begin{cases} \langle R_2, R_0 \rangle_w = \displaystyle\int_a^b w(x)(x^2 + a_{2,1}x + a_{2,0})\, dx = 0 \\ \langle R_2, R_1 \rangle_w = \displaystyle\int_a^b w(x)(x + a_{1,0})(x^2 + a_{2,1}x + a_{2,0})\, dx = 0 \end{cases}$$

If we denote $\mu_k = \int_a^b x^k w(x)\, dx$ then the coefficients $a_{2,0}, a_{2,1}$ are determined by

$$\begin{pmatrix} \mu_0 & \mu_1 \\ \mu_1 & \mu_2 \end{pmatrix} \begin{pmatrix} a_{2,0} \\ a_{2,1} \end{pmatrix} = - \begin{pmatrix} \mu_2 \\ \mu_3 \end{pmatrix}$$

which gives $a_{2,0}, a_{2,1}$ provided that the determinant

$$\Delta_2 := \begin{vmatrix} \mu_0 & \mu_1 \\ \mu_1 & \mu_2 \end{vmatrix} \neq 0.$$

Orthogonalisation Procedure (Doman, 2016)

Continuing this process, we define

$$R_n(x) = x^n + \sum_{k=0}^{n-1} a_{n,k} x^k$$

and use the orthogonality relations with $R_0, R_1, \ldots, R_{n-1}$, $(R_n \perp R_{n-1}, \ldots, R_n \perp R_0)$. That is

$$\langle R_n, R_k \rangle_w = \int_a^b w(x) R_n(x) R_k(x)\, dx = 0, \; k < n$$

These equations can be written in matrix form

$$\begin{pmatrix} \mu_0 & \mu_1 & \cdots & \mu_{n-1} \\ \mu_1 & \mu_2 & \cdots & \mu_n \\ \vdots & \vdots & \ddots & \vdots \\ \mu_{n-1} & \mu_n & \cdots & \mu_{2n-2} \end{pmatrix} \begin{pmatrix} a_{n,0} \\ a_{n,1} \\ \vdots \\ a_{n,n-1} \end{pmatrix} = - \begin{pmatrix} \mu_n \\ \mu_{n+1} \\ \vdots \\ \mu_{2n-1} \end{pmatrix}$$

Orthogonalisation Procedure (Doman, 2016)

The system will have a unique solution provided that

$$\Delta_{n-1} := \begin{vmatrix} \mu_0 & \mu_1 & \dots & \mu_{n-1} \\ \mu_1 & \mu_2 & \dots & \mu_n \\ \vdots & \vdots & \ddots & \vdots \\ \mu_{n-1} & \mu_n & \dots & \mu_{2n-2} \end{vmatrix} \neq 0$$

We can represent the transformation from the functions $1, x, \dots, x^n$ to $R_0(x), R_1(x), \dots, R_n(x)$ by the matrix transformation

$$\begin{pmatrix} R_0(x) \\ R_1(x) \\ R_2(x) \\ \vdots \\ R_n(x) \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 & \dots & 0 \\ a_{1,0} & 1 & 0 & \dots & 0 \\ a_{2,0} & a_{2,1} & 1 & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ a_{n,0} & a_{n-1,0} & a_{n-2,0} & \dots & 1 \end{pmatrix} \begin{pmatrix} 1 \\ x \\ x^2 \\ \vdots \\ x^n \end{pmatrix}$$

The polynomial R_n has n distinct real zeros in the interval (a, b).

Kernel Polynomial (Dahlquist and Björk,2008)

Let $R_n(x) = k_n x^n + \ldots, n = 0, 1, \ldots$ be a family of real orthogonal polynomials. The symmetric function

$$K_n(x, y) = \sum_{k=0}^{n} R_k(x) R_k(y)$$

is called the *kernel polynomial* of order n for the orthogonal system. For every polynomial $P \in \Pi_n$

$$\int P(x) K_n(x, y)\, dx = P(y).$$

Moreover,

$$K_n(x, y) = \frac{k_n}{k_{n+1}} \frac{R_{n+1}(x) R_n(y) - R_n(x) R_{n+1}(y)}{x - y}.$$

Classical Orthogonal Polynomials (Doman, 2016)

Fundamental interval and weight functions of the classical orthogonal polynomials can be separated into three distinct groups:

Hermite polynomials, H_n: $(a, b) = (-\infty, +\infty)$, $w(x) = e^{-x^2}$

Laguerre polynomials, $L_n^{(\alpha)}$: $(a, b) = (0, +\infty)$,
$w(x) = x^\alpha e^{-x}$, $\alpha > -1$

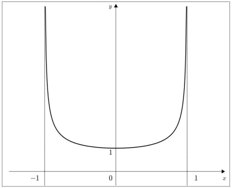
Jacobi polynomials, $P_n^{(\alpha,\beta)}$: $(a, b) = (-1, 1)$,
$w(x) = (1 - x)^\alpha (1 + x)^\beta$, $\alpha, \beta > -1$

The interval $(-1, 1)$ can be transformed to (a, b) as follows

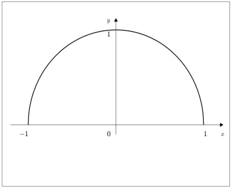
$$x = \frac{a + b}{2} + \frac{b - a}{2}\xi \in (a, b),\ \xi \in (-1, 1).$$

Weight Function

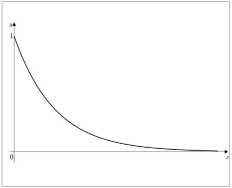
$w(x) = 1/\sqrt{1-x^2}$



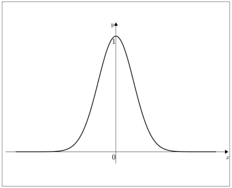
$w(x) = \sqrt{1-x^2}$



$w(x) = e^{-x}$



$w(x) = e^{-x^2}$



Hermite Polynomials (Doman, 2016)

Hermite polynomials are defined in two different ways by different classes of users. For the physicists, Hermite polynomials denoted by $H_n(x)$ arise from the orthogonalisation process for polynomials defined over a domain $(-\infty, \infty)$ with a weight function $w(x) = e^{-x^2}$. The probabilists define the Hermite polynomials, commonly denoted by $He_n(x)$, over the domain $(-\infty, \infty)$ with the weight function $w(x) = e^{-\frac{x^2}{2}}$. The two functions are related by

$$H_n(x) = \sqrt{2^n} He_n(\sqrt{2}x).$$

$$H_n(x) = (-1)^n e^{x^2} \frac{d^n}{dx^n}(e^{-x^2}), \ x \in \mathbb{R}.$$

Hermite Polynomials (Doman, 2016)

Recurrence relation

$$\begin{cases} H_0(x) = 1,\ H_1(x) = 2x \\ H_{n+1}(x) = 2xH_n(x) - 2nH_{n-1}(x) \end{cases}$$

$$H'(x) = 2nH_n(x)$$

$$\int_{-\infty}^{\infty} e^{-x^2} H_n(x) H_m(x)\, dx = \begin{cases} 0,\ m \neq n \\ 2^n n! \sqrt{\pi},\ m = n \end{cases}$$

The Hermite polynomials are orthogonal with respect to the weight function $w(x) = e^{-x^2}$.
The differential equation satisfied by Hermite polynomials is

$$y''(x) - 2xy'(x) + \lambda y(x) = 0.$$

Generalized Laguerre Polynomials (Doman, 2016)

The Generalized Laguerre polynomials $L_n^{(\alpha)}(x)$ arise from the orthogonalisation process for polynomials defined over a domain $(0, +\infty)$ with a weight function $w(x) = x^\alpha e^{-x}$, $\alpha > -1$. When $\alpha = 0$ $(w(x) = e^{-x})$, the polynomials are called Laguerre polynomials $L_n(x)$.

The weight function $w(x) = x^\alpha e^{-x}$ can be thought of as arising as a limit from the weight function $(x-a)^\alpha (b-x)^\beta$ by firstly putting $a = 0$, dividing through by b and putting $\beta = b$ to obtain $x^\alpha (1 - \frac{x}{b})^b$ and then taking the limit $b \to +\infty$.

Generalized Laguerre Polynomials (Doman, 2016)

$$L_n^{(\alpha)}(x) = \frac{1}{n!} x^{-\alpha} e^x \frac{d^n}{dx^n}(e^{-x} x^{\alpha+n}),\ x \in (0, \infty).$$

Recurrence relation

$$\begin{cases} L_0^{(\alpha)}(x) = 1,\ L_1^{(\alpha)}(x) = 1 - x \\ (n+1)L_{n+1}^{(\alpha)}(x) = (2n + \alpha + 1 - x)L_n^{(\alpha)}(x) - (n+\alpha)L_{n-1}^{(\alpha)}(x) \end{cases}$$

$$\int_0^\infty x^\alpha e^{-x} L_n^{(\alpha)}(x) L_m^{(\alpha)}(x)\, dx = \begin{cases} 0,\ m \neq n \\ \frac{\Gamma(\alpha+n+1)}{n!},\ m = n \end{cases}$$

The Laguerre polynomials are orthogonal with respect to the weight function $w(x) = x^\alpha e^{-x}$.

The differential equation satisfied by Laguerre polynomials is

$$xy''(x) + (\alpha + 1 - x)y'(x) + \lambda y(x) = 0.$$

Legendre Polynomials (Doman, 2016)

$$P_n(x) = \frac{1}{2^n n!} \frac{d^n}{dx^n}(x^2 - 1), \; x \in (-1, 1)$$

Recurrence relation

$$\begin{cases} P_0(x) = 1, \; P_1(x) = x \\ (n+1)P_{n+1}(x) = (2n+1)xP_n(x) - nP_{n-1}(x) \end{cases}$$

$$\int_{-1}^{1} P_n(x) P_m(x) \, dx = \begin{cases} 0, \; m \neq n \\ \frac{2}{2n+1}, \; m = n \end{cases}$$

The Legendre polynomials are orthogonal with respect to the weight function $w(x) = 1$.
The differential equation satisfied by Legendre polynomials is

$$(1 - x^2)y''(x) - 2xy'(x) + \lambda y = 0.$$

Chebyshev Polynomials of the first kind (Burden *et al.*,2022)

$$T_n(x) = \cos(n \arccos x), \quad x \in [-1, 1]$$

Recurrence relation

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

T_n is a polynomial of degree n with leading coefficient 2^{n-1}.

$$\int_{-1}^{1} \frac{1}{\sqrt{1-x^2}} T_n(x) T_m(x)\, dx = \begin{cases} 0, & m \neq n \\ \frac{\pi}{2}, & m = n \end{cases}$$

The Chebyshev polynomials of the first kind are orthogonal with respect to the weight function $w(x) = \frac{1}{\sqrt{1-x^2}}$.

Chebyshev Polynomials of the first kind (Rivlin, 1974)

$$
\begin{aligned}
T_0(x) &= 1, \\
T_1(x) &= x, \\
T_2(x) &= 2x^2 - 1, \\
T_3(x) &= 4x^3 - 3x, \\
T_4(x) &= 8x^4 - 8x^2 + 1, \\
T_5(x) &= 16x^5 - 20x^3 + 5x.
\end{aligned}
$$

Chebyshev Polynomials of the first kind (Rivlin, 1974)

$$T_n'(x) = n\frac{\sin(n\theta)}{\sin\theta},\; x = \cos\theta$$

$$|T_n(x)| \leqslant 1, \quad |T'(x)| \leqslant n^2$$

$$T_m(T_n(x)) = T_{mn}(x)$$

$$\int T_n(x)\,dx = \frac{1}{2}\Big(\frac{T_{n+1}(x)}{n+1} - \frac{T_{n-1}(x)}{n-1}\Big)$$

$$T_n(-x) = (-1)^n T_n(x)$$

$$(1-x^2)\,T_n'(x) = n\Big(T_{n-1}(x) - xT_n(x)\Big)$$

Chebyshev Polynomials of the first kind (Burden *et al.*,2022)

The differential equation satisfied by Chebyshev I polynomials is

$$(1 - x^2)y''(x) - xy'(x) + \lambda y(x) = 0$$

The Chebyshev polynomial $T_n(x)$ of degree $n > 1$ has n simple zeros in $[-1, 1]$ at

$$\bar{x}_k = \cos \frac{2k - 1}{2n}\pi, \quad k = \overline{1, n}.$$

Moreover, $T_n(x)$ assumes its absolute extrema (zeros of T_n' and ± 1) at

$$\bar{x}_k' = \cos \frac{k\pi}{n} \text{ with } T(\bar{x}_k') = (-1)^k, \quad k = \overline{0, n}.$$

Chebyshev Polynomials of the first kind (Burden *et al.*,2022)

The monic (polynomials with leading coefficient 1) Chebyshev polynomials $\tilde{T}_n(x)$ are derived from the Chebyshev polynomials $T_n(x)$ by dividing by the leading coefficient 2^{n-1}

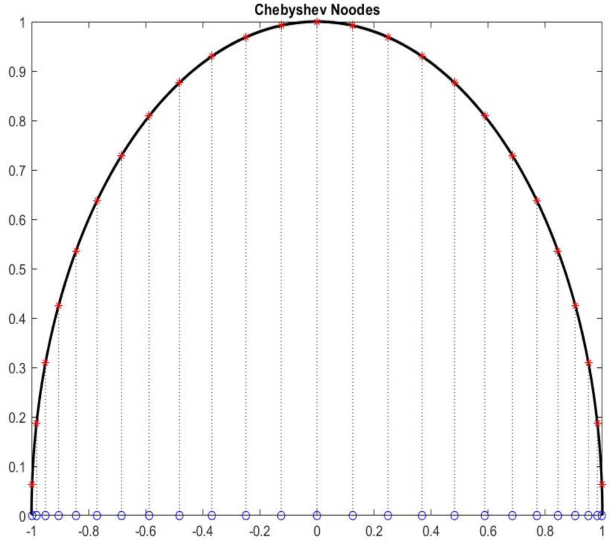
$$\tilde{T}_0(x) = 1, \quad \tilde{T}_n(x) = \frac{1}{2^{n-1}} T_n(x), \quad n \geqslant 1.$$

$\widetilde{\Pi}_n$-the set of all monic polynomials of degree n

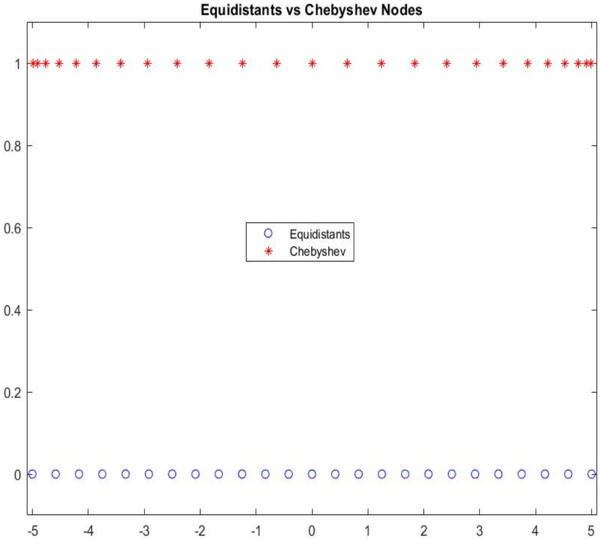
$$\frac{1}{2^{n-1}} = \max_{x \in [-1,1]} |\tilde{T}_n(x)| \leqslant \max_{x \in [-1,1]} |P_n(x)| \quad \forall\, P_n \in \widetilde{\Pi}_n$$

Moreover, equality occurs when $P_n = \tilde{T}_n$

Chebyshev Nodes



Chebyshev Nodes vs Equidistant Nodes



Chebyshev Polynomials of the second kind (Doman, 2016)

$$U_n(x) = \frac{\sin((n+1)\arccos x)}{\sin(\arccos x)},\ x \in [-1, 1]$$

Recurrence relations

$$\begin{cases} U_0(x) = 1,\ U_1(x) = 2x \\ U_{n+1}(x) = 2xU_n(x) - U_{n-1}(x) \end{cases}$$

$$U_n(x) = \frac{1}{n+1} T'_{n+1}(x)$$

$$\int_{-1}^{1} \sqrt{1-x^2}\, U_n(x) U_m(x)\, dx = \begin{cases} 0,\ m \neq n \\ \frac{\pi}{2},\ m = n \end{cases}$$

The Chebyshev polynomials of the second kind are orthogonal with respect to the weight function $w(x) = \sqrt{1-x^2}$.
The differential equation satisfied by Chebyshev II polynomials is

$$(1-x^2)y''(x) - 3xy'(x) + \lambda y(x) = 0.$$

Chebyshev Polynomials of the second kind (Rivlin, 1974)

$$
\begin{aligned}
U_0(x) &= 1, \\
U_1(x) &= x, \\
U_2(x) &= 4x^2 - 1, \\
U_3(x) &= 8x^3 - 4x, \\
U_4(x) &= 16x^4 - 12x^2 + 1, \\
U_5(x) &= 32x^5 - 32x^3 + 6x.
\end{aligned}
$$

Jacobi Polynomials (Doman, 2016)

$$P_n^{(\alpha,\beta)}(x) = \frac{(-1)^n}{2^n n!}(1-x)^{-\alpha}(1+x)^{-\beta}\frac{d^n}{dx^n}\left((1-x)^{n+\alpha}(1+x)^{n+\beta}\right)$$

$$\int_{-1}^{1}(1-x)^{\alpha}(1+x)^{\beta}P_m^{(\alpha,\beta)}(x)P_n^{(\alpha,\beta)}(x)\,dx = 0,\ m \neq n$$

$$\int_{-1}^{1}(1-x)^{\alpha}(1+x)^{\beta}\left(P_n^{(\alpha,\beta)}(x)\right)^2 dx =$$
$$= \frac{2^{\alpha+\beta+1}}{n!(\alpha+\beta+2n+1)}\frac{\Gamma(\alpha+n+1)\Gamma(\beta+n+1)}{\Gamma(\alpha+\beta+n+1)}$$

The Jacobi polynomials are orthogonal with respect to the weight function $w(x) = (1-x)^{\alpha}(1+x)^{\beta}$.

Jacobi Polynomials (Doman, 2016)

The differential equation satisfied by Jacobi polynomials is

$$(1 - x^2)y''(x) + \big(\beta - \alpha - (\alpha + \beta + 2)x\big)y'(x) + \lambda y(x) = 0.$$

Some special cases of Jacobi polynomials:

Legendre polynomials: $\alpha = \beta = 0$, $w(x) = 1$, $P_n = P_n^{(0,0)}$

Chebyshev I: $\alpha = \beta = -\frac{1}{2}$, $T_n = P^{(-\frac{1}{2},-\frac{1}{2})}$

Chebyshev II: $\alpha = \beta = \frac{1}{2}$, $U_n = P_n^{(\frac{1}{2},\frac{1}{2})}$