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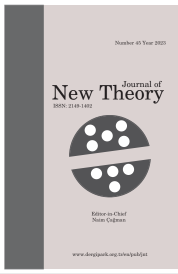

A Unified Approach to Computing the Zeros of Orthogonal Polynomials

Ridha Moussa[1], **James Tipton**[2]

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Abstract — We present a unified approach to calculating the zeros of the classical orthogonal polynomials and discuss the electrostatic interpretation and its connection to the energy minimization problem. This approach works for the generalized Bessel polynomials, including the normalized reversed variant, as well as the Vieté–Pell and Vieté–Pell–Lucas polynomials. We briefly discuss the electrostatic interpretation for each aforesaid case and some recent advances. We provide zeros and error estimates for various cases of the Jacobi, Hermite, and Laguerre polynomials and offer a brief discussion of how the method was implemented symbolically and numerically with Maple. In conclusion, we provide possible avenues for future research.

Keywords *Orthogonal polynomials, zeros, electrostatic interpretation*

Mathematics Subject Classification (2020) 33C45, 42C05

1. Introduction

The Jacobi, Hermite, and Laguerre polynomials are called classical orthogonal polynomials. They have served as objects of study as early as the 19th century and found applications in physics and approximation and number theory. For example, the Jacobi polynomials contain the Legendre polynomials as a special case, the coefficients in the expansion of the gravitational potential associated to a point mass [1]. The last two chapters of Szegö's classic text [2] focus on applications to interpolation and mechanical quadrature. More recently, the theory of orthogonal polynomials was used to present a formulation of quantum mechanics [3]. The classical orthogonal polynomials may be characterized as solutions to a Sturm–Liouville type equation of the form:

$$Q(x)y'' + L(x)y' + \lambda y = 0$$

In the case of the Jacobi polynomials, $Q(x) = 1-x^2$, $L(x) = \beta-\alpha-(\alpha+\beta+2)x$, and $\lambda = n(n+\alpha+\beta+1)$. For the Hermite polynomials, $Q(x) = 1$, $L(x) = -2x$, and $\lambda = 2n$. For the generalized Laguerre polynomials, $Q(x) = x$, $L(x) = (\alpha + 1 - x)$, and $\lambda = n$. In each case, the corresponding polynomial solutions satisfy an orthogonality condition of the form

$$\int_{-\infty}^{\infty} P_m(x)P_n(x)W(x)dx = 0, \quad m \neq n$$

[1]rmoussa@nsu.edu; [2]jetipton@nsu.edu (Corresponding Author)
[1,2]Department of Mathematics, College of Science, Engineering, and Technology, Norfolk State University, Norfolk, United States

where for the Jacobi polynomials,

$$W(x) = \begin{cases} (1-x)^{\alpha}(1+x)^{\beta}, & -1 \leq x \leq 1 \\ 0, & |x| > 1 \end{cases}$$

for the Hermite polynomials,

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

and for the generalized Laguerre polynomials,

$$W(x) = \begin{cases} x^{\alpha}e^{-x}, & x \geq 0 \\ 0, & x < 0 \end{cases}$$

Some topics of recent interest in the area of orthogonal polynomials include generalized Bessel polynomials [4], Vieté–Pell–Lucas polynomials [5, 6], and quasi-orthogonal polynomials [7]. Dunster et al. [4] study the reverse generalized Bessel polynomials by combining a qualitative analysis involving Liouville–Green Stokes lines and anti-Stokes lines with a fixed point method to calculate their zeros. Tasci and Yalcin [6] present some fundamental properties of Vieté–Pell and Vieté–Pell–Lucas polynomials, such as their characteristic equations, Binet formulas, and generating functions. More recently, Kuloğlu et al. [5] study a generalization of these polynomials, incomplete generalized Vieté–Pell and Vieté–Pell–Lucas polynomials, presenting recurrence relations and their generating functions. The well-known electrostatic interpretation is a central reason for continued interest in the zeros of classical and nonclassical orthogonal polynomials. Ismail [8, 9] extensively researches this topic, including a recent study on the general theory of quasi-orthogonal polynomials, which included an investigation into an electrostatic equilibrium problem [7]. Another point of interest is that these zeros have been used in quadrature rules [10–12].

The above treatment can be provided to both the (normalized reversed) generalized Bessel polynomials and the Vieté–Pell and Vieté–Pell–Lucas polynomials. Take $Q(x) = x^2$, $L(x) = \alpha x + \beta$, and $\lambda = -n(n+\alpha-1)$, for the generalized Bessel polynomials, while the normalized reverse Bessel polynomials satisfy $Q(x) = x$, $L(x) = -(2n-2+a+2x)$, and $\lambda = 2n$ (for more details, see [4, 13]). To provide Vieté–Pell and Vieté–Pell–Lucas polynomials a similar treatment, one can exploit their relationship to the Chebyshev polynomials to find that $Q(x) = 4-x^2$, $L(x) = -3x$, and $\lambda = n(n+1)$ for the Vieté–Pell polynomials and $Q(x) = 4-x^2$, $L(x) = -x$, and $\lambda = n^2$ for the Vieté–Pell–Lucas polynomials.

We present a unified method to calculate the zeros of a class of orthogonal polynomials, including the classical orthogonal polynomials and generalized Bessel polynomials. We discuss the electrostatic interpretation for several cases and the connection to the energy minimization problem. The method in question differs from that used by Dunster et al. [4] and is more akin to an approach developed by Pasquini [14–16] and more recently [17]. In Section 2, we present the details of the method. In Section 3, we discuss the electrostatic interpretation in the context of the energy minimization problem. We briefly outline how to implement the method symbolically and numerically in Section 4. In Section 5, we provide some examples. The paper concludes with possible avenues for future investigation.

2. Method

Given a polynomial $y = c_n \prod_{i=1}^{n}(x-x_i)$, where $c_n, x_i \in \mathbb{R}$, $c_n \neq 0$, and the x_i are distinct,

$$\frac{y'}{y} = \sum_{i=1}^{n} \frac{1}{x-x_i} \tag{1}$$

$$\frac{y''}{y} = \sum_{i=1}^{n}\sum_{j\in J_i}\frac{1}{(x-x_i)(x-x_j)} = 2\sum_{i<j}\frac{1}{(x-x_i)(x-x_j)} \tag{2}$$

and

$$\frac{ax^2+bx+c}{(x-x_i)(x-x_j)} = a + \frac{ax_i^2+bx_i+c}{(x_i-x_j)(x-x_i)} + \frac{ax_j^2+b_j+c}{(x_j-x_i)(x-x_j)} \tag{3}$$

where J_i consists of all integers in $[1,n]$ except i. Identities 1 and 2 follow from the product rule. Identity 3 follows from partial fraction decomposition.

Lemma 2.1. From the above setting,

$$(\mu x+\nu)\frac{y'}{y} = \mu n + \sum_{i=1}^{n}\frac{\nu+\mu x_i}{x-x_i}$$

and

$$(ax^2+bx+c)\frac{y''}{y} = a(n^2-n) + 2\sum_{i\neq j}\frac{ax_i^2+bx_i+c}{(x_i-x_j)(x-x_i)}$$

PROOF.
The first identity follows directly from Identity 1 and some long division. For the second identity, combine Identities 2 and 3 and get the equality

$$(ax^2+bx+c)\frac{y''}{y} = 2\sum_{i<j}\left[a + \frac{ax_i^2+bx_i+c}{(x_i-x_j)(x-x_i)} + \frac{ax_j^2+bx_j+c}{(x_j-x_i)(x-x_j)}\right]$$

There are $\frac{n^2-n}{2}$ terms in the above summation. Thus, $2\sum\limits_{i<j} a = a(n^2-n)$. Observe that

$$\begin{aligned}\sum_{i<j}\left[\frac{ax_i^2+bx_i+c}{(x_i-x_j)(x-x_i)} + \frac{ax_j^2+bx_j+c}{(x_j-x_i)(x-x_j)}\right] &= \sum_{i<j}\frac{ax_i^2+bx_i+c}{(x_i-x_j)(x-x_i)} + \sum_{i<j}\frac{ax_j^2+bx_j+c}{(x_j-x_i)(x-x_j)}\\ &= \sum_{i<j}\frac{ax_i^2+bx_i+c}{(x_i-x_j)(x-x_i)} + \sum_{j<i}\frac{ax_i^2+bx_i+c}{(x_i-x_j)(x-x_i)}\\ &= \sum_{i\neq j}\frac{ax_i^2+bx_i+c}{(x_i-x_j)(x-x_i)}\end{aligned}$$

where the second to last equality follows from index swapping on the second summation. Putting the above calculations together yields the desired result. □

Proposition 2.2. Suppose y is a degree n polynomial solution to the differential equation

$$(ax^2+bx+c)y'' + (\mu x+\nu)y' + \kappa y = 0$$

If the zeros of y, x_1, $\cdots$, x_n are distinct, then for each integer $k \in [1,n]$,

$$2\sum_{j\in J_k}\frac{ax_k^2+bx_k+c}{x_k-x_j} + \nu + \mu x_k = 0$$

PROOF.
Divide by y and apply Lemma 1,

$$a(n^2-n)+2\sum_{i\neq j}\frac{ax_i^2+bx_i+c}{(x_i-x_j)(x-x_i)}+\mu n+\sum_{i=1}^{n}\frac{\nu+\mu x_i}{x-x_i}+\kappa=0 \Leftrightarrow 2\sum_{i\neq j}\frac{ax_i^2+bx_i+c}{(x_i-x_j)(x-x_i)}+\sum_{i=1}^{n}\frac{\nu+\mu x_i}{x-x_i}+M=0$$

$$\Leftrightarrow 2(x-x_k)\sum_{i\neq j}\frac{ax_i^2+bx_i+c}{(x_i-x_j)(x-x_i)}$$

$$+(x-x_k)\sum_{i=1}^{n}\frac{\nu+\mu x_i}{x-x_i}+(x-x_k)M=0$$

where $M=\kappa+a(n^2-n)+\mu n$ and k is some integer in $[1,n]$. As x approaches x_k, all terms will approach zero except those for $i=k$. Taking this limit gives the desired result. $\square$

2.1. Jacobi Polynomials

For $\alpha,\beta>-1$, the degree n Jacobi polynomial $P_n^{(\alpha,\beta)}(x)$ solves the differential equation

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

Denote the n distinct zeros of $P_n^{(\alpha,\beta)}(x)$ by $x_1,\cdots,x_n$. Let $a=-1$, $b=0$, $c=1$, $\mu=-(\alpha+\beta+2)$, and $\nu=\beta-\alpha$. By Proposition 2.2, we see that the zeros must satisfy

$$2\sum_{j\in J_k}\frac{-x_k^2+1}{x_k-x_j}+\beta-\alpha-(\alpha+\beta+2)x_k=0\Leftrightarrow\frac{\frac{1}{2}(\alpha+1)}{x_k-1}+\frac{\frac{1}{2}(\beta+1)}{x_k+1}+\sum_{j\in J_k}\frac{1}{x_k-x_j}=0 \tag{4}$$

The following theorem, which we have adapted from the Marsden and Hoffman classic [18], expresses the well-known fact that a continuous real-valued function over a compact set must attain an absolute maximum:

Theorem 2.3. [18] Suppose $A\subset\mathbb{R}^n$ and let $f:A\to\mathbb{R}$ be continuous. If $K\subset A$ is compact, then f is bounded on K. Furthermore, there exists an $x_0\in K$ such that $f(x_0)=\sup f(A)$.

In what follows, consider the real-valued function

$$f(\vec{x})=\prod_{k=1}^{n}\left[(1-x_k)^{(\alpha+1)/2}(1+x_k)^{(\beta+1)/2}\right]\prod_{i<j}(x_j-x_i)$$

defined over the set $D_n=\{\vec{x}\in\mathbb{R}^n:-1<x_1<x_2<\cdots<x_n<1\}$. Note that f is smooth over D_n and continuous on $\overline{D_n}$. Note that f vanishes on the boundary of D_n but is positive over D_n. Since f must attain an absolute maximum in $\overline{D_n}$, the previous observations show that this maximum occurs in D_n and must be a critical point.

Lemma 2.4. A point $\vec{x}\in D_n$ is a critical point of f if and only if Expression 4 holds for $k\in\{1,2,3,\cdots,n\}$.

Proof.
Consider instead

$$\ln(f)=\sum_{k=1}^{n}\left[\frac{\alpha+1}{2}\ln(1-x_k)+\frac{\beta+1}{2}\ln(1+x_k)\right]+\sum_{i<j}\ln(x_j-x_i)$$

we have that

$$\frac{\partial\ln(f)}{\partial x_k}=\frac{f_{x_k}}{f}=\frac{\frac{1}{2}(\alpha+1)}{x_k-1}+\frac{\frac{1}{2}(\beta+1)}{x_k+1}+\sum_{j\in J_k}\frac{1}{x_k-x_j}$$

demonstrating the claim. $\square$

Lemma 2.5. The function $\ln(f)$ has only one critical point in D_n.

Proof.
The claim holds if we can show that $\ln(f)$ is concave in D_n. This, in turn, will follow if we can show that the Hessian of $\ln(f)$ is diagonally dominant and negative definite. To that extent, observe that

$$\frac{\partial^2 \ln(f)}{\partial x_k^2} = \frac{-\frac{1}{2}(\alpha+1)}{(x_k-1)^2} - \frac{\frac{1}{2}(\beta+1)}{(x_k+1)^2} - \sum_{j\in J_k} \frac{1}{(x_k-x_j)^2}$$

and for $i \neq j$ that

$$\frac{\partial^2 \ln(f)}{\partial x_i x_j} = \frac{1}{(x_i-x_j)^2}$$

The Hessian is thus diagonally dominant and negative definite. □

Example 2.6. To see the above results in action, set $\alpha = \beta = 0$, giving the Legendre differential equation:

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

The general solution is

$$y = k_1 P_n(x) + k_2 Q_n(x)$$

where

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

is the n-th Legendre polynomial and

$$Q_n = \begin{cases} \frac{1}{2}\log\frac{1+x}{1-x}, & \text{if } n=0 \\ P_1(x)Q_0(x) - 1, & \text{if } n=1 \\ \frac{2n-1}{n}Q_{n-1}(x) - \frac{n-1}{n}Q_{n-2}(x), & \text{if } n \geq 2 \end{cases}$$

is the n-th Legendre function of the second kind [2]. For $n = 2$, the second Legendre polynomial $P_2(x) = \frac{3x^2-1}{2}$ solves the following differential equation:

$$(1-x^2)y'' - 2xy' + 6y = 0$$

The corresponding real-valued function on D_2 is

$$f(x_1, x_2) = (x_2 - x_1)\sqrt{(1-x_1^2)(1-x_2^2)}$$

which attains a global maximum at $x_1 = -1/\sqrt{3}$ and $x_2 = 1/\sqrt{3}$. It is clear that $P_2(x_1) = P_2(x_2) = 0$.

2.2. Hermite Polynomials

The degree n Hermite polynomial $H_n(x)$ solves the differential equation $y'' - 2xy^{'} + 2ny = 0$. Denote the n distinct zeros of $H_n(x)$ by $x_1, \cdots, x_n$. Let $a = b = \nu = 0$, $c = 1$, $\mu = -2$, and $\kappa = 2n$. By Proposition 2.2, we observe that the zeros must satisfy

$$2\sum_{j\in J_k}\frac{1}{x_k-x_j} - 2x_k = 0 \Leftrightarrow \sum_{j\in J_k}\frac{1}{x_k-x_j} - x_k = 0 \tag{5}$$

In what follows, consider the real-valued function

$$f(\vec{x}) = \prod_{i<j}\Big[x_j - x_i\Big]e^{-\frac{1}{2}\sum_{k=1}^{n}x_k^2}$$

defined over the set $D_n = \{\vec{x} \in \mathbb{R}^n : -\infty < x_1 < x_2 < \cdots < x_n < \infty\}$. Note that f is smooth, positive and bounded over D_n but approaches 0 on the boundary. Thus, f must have a critical point in D_n.

Lemma 2.7. A point $\vec{x} \in D_n$ is a critical point of f if and only if Expression 5 holds for $k \in \{1, 2, 3, \cdots, n\}$.

PROOF.
Consider instead

$$\ln(f) = \sum_{i<j} \ln(x_j - x_i) - \frac{1}{2} \sum_{k=1}^{n} x_k^2$$

we have that

$$\frac{\partial \ln(f)}{\partial x_k} = \frac{f_{x_k}}{f} = \sum_{j \in J_k} \frac{1}{x_k - x_j} - x_k$$

demonstrating the claim. □

Lemma 2.8. The function $\ln(f)$ has only one critical point in D_n.

PROOF.
The claim holds if we can show that $\ln(f)$ is concave in D_n. This, in turn, will follow if we can show that the Hessian of $\ln(f)$ is diagonally dominant and negative definite. To that extent, observe that

$$\frac{\partial^2 \ln(f)}{\partial x_k^2} = -\sum_{j \in J_k} \frac{1}{(x_k - x_j)^2} - 1$$

and for $i \neq j$ that

$$\frac{\partial^2 \ln(f)}{\partial x_i x_j} = \frac{1}{(x_i - x_j)^2}$$

The Hessian is thus diagonally dominant and negative definite. □

2.3. Laguerre Polynomials

The degree n generalized Laguerre polynomial $L_n^{(\alpha)}(x)$ solves the differential equation

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

Denote the n distinct zeros of $L_n^{(\alpha)}(x)$ by $x_1, \cdots, x_n$. Let $a = c = 0$, $b = 1$, $\mu = -1$, $\nu = \alpha + 1$, and $\kappa = n$. By Proposition 2.2, we see that the zeros must satisfy

$$2 \sum_{j \in J_k} \frac{x_k}{x_k - x_j} + \alpha + 1 - x_k = 0 \Leftrightarrow \sum_{j \in J_k} \frac{1}{x_k - x_j} + \frac{\frac{1}{2}(\alpha + 1)}{x_k} - \frac{1}{2} = 0 \tag{6}$$

In what follows, consider the real-valued function

$$f(\vec{x}) = \prod_{i<j} \left[x_j - x_i\right] \prod_{k=1}^{n} \left[x_k^{(\alpha+1)/2}\right] e^{-\frac{1}{2}\sum_{k=1}^{n} x_k}$$

defined over the set $D_n = \{\vec{x} \in \mathbb{R}^n : 0 < x_1 < x_2 < \cdots < x_n < \infty\}$. Note that f is smooth, positive and bounded over D_n but approaches 0 on the boundary. Thus, f must have a critical point in D_n.

Lemma 2.9. A point $\vec{x} \in D_n$ is a critical point of f if and only if Expression 6 holds for $k \in \{1, 2, 3, \cdots, n\}$.

PROOF.
Consider instead

$$\ln(f) = \sum_{i<j} \ln(x_j - x_i) + \sum_{k=1}^{n} \left[\frac{\alpha + 1}{2} \ln x_k\right] - \frac{1}{2} \sum_{k=1}^{n} x_k$$

we have that

$$\frac{\partial \ln(f)}{\partial x_k} = \frac{f_{x_k}}{f} = \sum_{j \in J_k} \frac{1}{x_k - x_j} + \frac{\frac{1}{2}(\alpha+1)}{x_k} - \frac{1}{2}$$

demonstrating the claim. □

Lemma 2.10. The function $\ln(f)$ has only one critical point in D_n.

PROOF.
The claim holds if we can show that $\ln(f)$ is concave in D_n. This, in turn, will follow if we can show that the Hessian of $\ln(f)$ is diagonally dominant and negative definite. To that extent, observe that

$$\frac{\partial^2 \ln(f)}{\partial x_k^2} = -\sum_{j \in J_k} \frac{1}{(x_k - x_j)^2} - \frac{\frac{1}{2}(\alpha+1)}{x_k^2} < 0$$

and for $i \neq j$ that

$$\frac{\partial^2 \ln(f)}{\partial x_i x_j} = \frac{1}{(x_i - x_j)^2}$$

The Hessian is thus diagonally dominant and negative definite. □

2.4. Normalized Reversed Generalized Bessel Polynomials

The normalized reversed generalized Bessel polynomials (RGBP)

$$\hat{\theta}_n(z;a) = \theta_n\left(\frac{(2n+a-2)z}{2};a\right)$$

satisfy the differential equation

$$\frac{2z}{2n+a-2}\hat{\theta}_n'' - (2z+2)\hat{\theta}_n' + 2n\hat{\theta}_n = 0$$

Applying Proposition 2.2,

$$\sum_{j \in J_k} \frac{1}{z_k - z_j} + \frac{M_{n,a}}{z_k} + M_{n,a} = 0 \tag{7}$$

where $M_{n,a} = \dfrac{2-2n-a}{2}$, which correspond to the critical points of the function

$$f(\vec{z}) = \prod_{i<j}(z_j - z_i) \prod_{i=1}^{n}\left(z_i^{M_{n,a}}\right) e^{M_{n,a}\sum z_i}$$

with domain $D_n = \{\vec{z} : z_i \neq z_j \text{ if } i \neq j\}$.

Lemma 2.11. A point $\vec{z} \in D_n$ is a critical point of f if and only if Equation 7 holds for $k \in \{1,2,3,\cdots,n\}$.

PROOF.
Consider instead

$$\ln(f) = \sum_{i<j} \ln(z_j - z_i) + M_{n,a}\sum_{i=1}^{n} \ln z_i - M_{n,a}\sum_{i=1}^{n} z_k$$

we have that

$$\frac{\partial \ln(f)}{\partial z_k} = \frac{f_{z_k}}{f} = \sum_{j \in J_k} \frac{1}{z_k - z_j} + \frac{M_{n,a}}{z_k} - M_{n,a}$$

demonstrating the claim. □

Lemma 2.12. The function $\ln(f)$ has only one critical point in D_n.

Proof.
The claim holds if we can show that $\ln(f)$ is concave in D_n. This, in turn, will follow if we can show that the Hessian of $\ln(f)$ is diagonally dominant and negative definite. To that extent, observe that

$$\frac{\partial^2 \ln(f)}{\partial z_k^2} = -\sum_{j\in J_k} \frac{1}{(z_k - z_j)^2} - \frac{M_{n,a}}{z_k^2}$$

and for $i \neq j$ that

$$\frac{\partial^2 \ln(f)}{\partial z_i z_j} = \frac{1}{(z_i - z_j)^2}$$

The Hessian is thus diagonally dominant and negative definite. □

2.5. Generalized Bessel Polynomials

In the case of generalized Beesel Polynomials (GBP), which satisfies the differential equation $x^2y'' + (\alpha x + \beta)y' + n(n + \alpha - 1)y = 0$, we can take $a = 1$, $b = c = 0$, $\mu = \alpha$, $\nu = \beta$, and $\kappa = n(n + \alpha - 1)$, to get that the zeros of the nth GBP satisfy

$$\sum_{j\in J_k} \frac{1}{x_k - x_j} + \frac{\frac{1}{2}\beta}{x_k^2} + \frac{\frac{1}{2}\alpha}{x_k} = 0 \tag{8}$$

These correspond to the critical points of the function

$$f(\vec{x}) = \prod_{i<j} (x_j - x_i) \prod_{i=1}^{n} \left(x_i^{\alpha/2}\right) e^{-\frac{1}{2}\beta \sum 1/x_i}$$

with domain $D_n = \{\vec{x} : x_i \neq x_j \text{ if } i \neq j\}$.

Lemma 2.13. A point $\vec{x} \in D_n$ is a critical point of f if and only if Equation 8 holds for $k \in \{1, 2, 3, \cdots, n\}$.

Proof.
Consider instead

$$\ln(f) = \sum_{i<j} \ln(x_j - x_i) + \frac{\alpha}{2}\sum_{i=1}^{n} \ln x_i - \frac{\beta}{2}\sum_{i=1}^{n} \frac{1}{x_i}$$

we have that

$$\frac{\partial \ln(f)}{\partial x_k} = \frac{f_{x_k}}{f} = \sum_{j\in J_k} \frac{1}{x_k - x_j} + \frac{\frac{1}{2}\alpha}{x_k} + \frac{\frac{1}{2}\beta}{x_k^2}$$

demonstrating the claim. □

Lemma 2.14. The function $\ln(f)$ has only one critical point in D_n.

Proof.
The claim holds if we can show that $\ln(f)$ is concave in D_n. This, in turn, will follow if we can show that the Hessian of $\ln(f)$ is diagonally dominant and negative definite. To that extent, observe that

$$\frac{\partial^2 \ln(f)}{\partial x_k^2} = -\sum_{j\in J_k} \frac{1}{(x_k - x_j)^2} - \frac{\frac{1}{2}\alpha}{x_k^2} - \frac{\frac{1}{2}\beta}{x_k^2}$$

and for $i \neq j$ that

$$\frac{\partial^2 \ln(f)}{\partial x_i x_j} = -\sum_{j\in J_k} \frac{1}{(x_i - x_j)^2}$$

The Hessian is thus diagonally dominant and negative definite. □

2.6. Vieté–Pell and Vieté–Pell–Lucas Polynomials

Vieté–Pell polynomials satisfy the differential equation $(4-x^2)y''-3xy'+n(n+1)y=0$ and Vieté–Pell–Lucas polynomials satisfy the differential equation $(4-x^2)y''-xy'+n^2y=0$ where n is the degree of the polynomial. Applying Proposition 2.2 in each case, we find that the zeros satisfy

$$\sum_{j\in J_k}\frac{1}{x_k-x_j}+\frac{\frac{3}{4}}{x_k+2}+\frac{\frac{3}{4}}{x_k-2}=0 \tag{9}$$

and

$$\sum_{j\in J_k}\frac{1}{x_k-x_j}+\frac{\frac{1}{2}}{x_k+2}+\frac{\frac{1}{2}}{x_k-2}=0 \tag{10}$$

respectively. Consider the functions

$$f(\vec{x})=\prod_{k=1}^{n}\left[(2-x_k)^{\frac{3}{4}}(2+x_k)^{\frac{3}{4}}\right]\prod_{i<j}(x_j-x_i)$$

and

$$g(\vec{x})=\prod_{k=1}^{n}\left[(2-x_k)^{\frac{1}{2}}(2+x_k)^{\frac{1}{2}}\right]\prod_{i<j}(x_j-x_i)$$

Proceeding as in the Jacobi case, one finds that:

Lemma 2.15. A point $\vec{x}\in D_n$ is a critical point of f (resp. g) if and only if Equation 9 (resp. Equation 10) holds for $k\in\{1,2,\cdots,n\}$.

PROOF.
Consider instead

$$\ln(f)=\sum_{i<j}\ln(x_j-x_i)+\frac{3}{4}\sum_{i=1}^{n}\ln(2-x_i)+\frac{3}{4}\sum_{i=1}^{n}\ln(2+x_i)$$

we have that

$$\frac{\partial\ln(f)}{\partial x_k}=\frac{f_{x_k}}{f}=\sum_{j\in J_k}\frac{1}{x_k-x_j}+\frac{\frac{3}{4}}{x_k-2}+\frac{\frac{3}{4}}{x_k+2}$$

demonstrating the claim for f. For g, replace $\frac{3}{4}$ with $\frac{1}{2}$. □

Lemma 2.16. The functions $\ln(f)$ and $\ln(g)$ have only one critical point in D_n.

PROOF.
The claim holds if we can show that both $\ln(f)$ and $\ln(g)$ are concave in D_n. This, in turn, will follow if we can show that their Hessians are diagonally dominant and negative definite. To that extent, observe that

$$\frac{\partial^2\ln(f)}{\partial x_k^2}=-\sum_{j\in J_k}\frac{1}{(x_k-x_j)^2}-\frac{\frac{3}{4}}{(x_k-2)^2}-\frac{\frac{3}{4}}{(x_k+2)^2}$$

and for $i\neq j$ that

$$\frac{\partial^2\ln(f)}{\partial x_i x_j}=-\sum_{j\in J_k}\frac{1}{(x_i-x_j)^2}$$

For g, replace $\frac{3}{4}$ with $\frac{1}{2}$. In either case, the Hessian is thus diagonally dominant and negative definite.
□

3. Electrostatic Interpretation and the Connection to the Energy Minimization Problem

As detailed by Szego in [2], the zeros of the classical orthogonal polynomials may be interpreted as the equilibrium position of an electrostatic problem. Stieltjes derived this connection in the case of the Jacobi polynomials in 1885. In this case, the problem is to find the position of $n \geq 2$ unit masses in the interval $[-1, 1]$ given two fixed positive masses $\frac{\alpha+1}{2}$ and $\frac{\beta+1}{2}$ at -1 and 1, respectively, for which electrostatic equilibrium is attained. The problem is solved by locating the zeros of the Jacobi polynomial $P_n^{(\alpha,\beta)}(x)$ [2]. Stieltjes provided a similar interpretation to the other classical orthogonal polynomials. The unit "masses" lie in the interval $(0, \infty)$ for the Laguerre polynomials with the restriction that the arithmetic mean of the unit charges is uniformly bounded and $(-\infty, \infty)$ for the Hermite polynomials with the restriction that the square arithmetic mean of the unit charges is uniformly bounded [2, 19].

A similar electrostatic interpretation may be presented for Vieté–Pell and Vieté–Pell–Lucas polynomials; the unit masses lie in the interval $[-2, 2]$, where we have positive mass $\frac{3}{4}$ at both -2 and 2 in Vieté–Pell case and positive mass $\frac{1}{2}$ at both -2 and 2 in Vieté–Pell–Lucas case. To the best of our knowledge, an electrostatic interpretation for the normalized RGBP and the GBP remains open. Interest in this connection has been steadily growing; see Marcellán, Martínez-Finkelshtein and Martínez-González's excellent survey [19] for details. As noted in [19], this is due in part to advances in the theory of logarithmic potentials as well as special functions from other areas of study, such as physics, combinatorics and number theory. Marcellán et al. [19] consider the following natural questions:

i. Can the electrostatic interpretation be generalized to other families of polynomials?

ii. Is it necessary to consider the global minimum of the energy? What about other equilibria?

In regards to the first question, it is noted in [19] that Ismail [8, 9] has provided an electrostatic model for general orthogonal polynomials, in which the external field is given as the sum of a long-range and short-range potential. For example, in [8], an explicit formula is given for the total energy of the model at the equilibrium position, and this energy is shown to be minimum. In the case of Freud weights, the total energy is shown to be asymptotic to $\frac{-n^2}{\alpha} \ln n$.

The authors [19] consider a more general case where the weight function satisfies the Pearson equation, particularly with the weight function corresponding to the Freud-type polynomials. It is noted that, in this case, the zeros of the Freud-type polynomials provide a critical configuration for the total energy. Still, it is an open problem whether the zeros are in a stable equilibrium. Regarding the second question, it is posited whether other types of equilibria are preserved in this case. The authors [19] present a max-min characterization of the zeros of the Jacobi polynomials, which is amenable to complex zeros of the family when the parameters fall out of the "classical" bounds. Loosely speaking, the characterization shows that of all possible compact continua from -1 to 1 (within the complex plane), the energy (minimized over n points for a given compact continua) is maximized over all compact continua when the n points are the zeros of the Jacobi polynomial.

More recently, regarding the first question above, Ismail and Wang developed an electrostatic interpretation of quasi-orthogonal polynomials in [7]. The main result is analogous to one given in [8]. In brief, it says that the equilibrium position of n unit charges in the presence of a given external field is uniquely attained at the zeros of the associated quasi-orthogonal polynomials.

4. Implementation

The above method was implemented using an amalgamation of symbolic and numerical approaches in Maple 2018. As an illustration, we present the steps taken to calculate the zeros of the Laguerre polynomial $L_9^{(0)}(x)$.

Step 1. We implement the initial guess procedure using the asymptotic formula in the Digital Library of Mathematical Functions section 18.16. [20]. The input for the initial guess procedure is α and n corresponding to the desired Laguerre polynomial $L_n^{(\alpha)}(x)$.

Step 2. We define the nonlinear system Expression 6, corresponding to the Laguerre polynomials.

Step 3. We calculate the Jacobian matrix using the built-in Maple function "Jacobian".

Step 4. For instructive purposes, we perform one iteration of Newton's method before writing a loop to iterate it ten times. We evaluate $L_9^{(0)}(x)$ at the approximated zeros as a quick check for accuracy. Maple produces the zeros after each iteration.

5. Illustrative Examples

In the following Tables 1-7, zeros approximations are listed for a variety of classical orthogonal polynomials of a specified degree n. The Jacobi column corresponds to the general Jacobi polynomial with $\alpha = \frac{1}{4}$ and $\beta = \frac{1}{8}$. The Chebyshev column refers to the Chebyshev polynomials of the 1st kind, which correspond to Jacobi polynomials with $\alpha = \beta = \frac{-1}{2}$. The Gegenbauer column corresponds to Jacobi polynomials with $\alpha = \beta = \frac{1}{4}$. The Legendre column corresponds to Jacobi polynomials with $\alpha = \beta = 0$. The Laguerre column corresponds to the classical Laguerre polynomials. The General Laguerre column corresponds to Laguerre polynomials with $\alpha = 1$.

These results are obtained by using a straightforward implementation of Newton's method in the following way: Let n be a fixed natural number and consider the vector $\vec{x} = (x_1, x_2, \cdots, x_n)$ which contains the zeros of the orthogonal polynomial of degree n and $\vec{f} = (f_1, f_2, \cdots, f_n)$ be a vector-valued function. With this notation, we can write the system of equations as $\vec{f}(\vec{x}) = \vec{0}$. The nonlinear equation above is represented by Expression 4 in the case of the Jacobi polynomials, by Expression 5 in the case of the generalized Laguerre polynomials and by Expression 6 in the case of the Hermite polynomials. As for the initial guess, we relied on formulas given in Section 18.16 of [20].

Since the exact roots are known for the Chebyshev case, one may calculate the exact error. Thus, the same can be said for Vieté–Pell and Vieté–Pell–Lucas polynomials. Using the infinity norm we have for $n = 20$ the exact error is 6.749×10^{-17}, while for $n = 25$ the exact error is 6.297×10^{-17}. We provide error estimates in each case using the infinity norm.

Table 1. Error estimates for $n = 20$

Polynomial	**Error Estimate**
Legendre	$1.6064700823479085388 \times 10^{-16}$
General Jacobi $\alpha = 1/4$, $\beta = 1/8$	$2.0443258006786251481 \times 10^{-16}$
Gegenbauer	$2.4276213934271014550 \times 10^{-16}$
Chebyshev 1st Kind	$2.775557561562891350 \times 10^{-17}$
Classical Laguerre	$7.0122389569333584353 \times 10^{-15}$
General Laguerre $\alpha = 1$	$1.0850726264919494635 \times 10^{-14}$
Hermite	$1.2572574676652352260 \times 10^{-16}$

Table 2. Error estimates for $n = 25$

Polynomial	**Error Estimate**
Legendre	$2.1554887097997079110 \times 10^{-16}$
General Jacobi $\alpha = 1/4$, $\beta = 1/8$	$1.1129640277756032144 \times 10^{-16}$
Gegenbauer	$1.4290762156055028002 \times 10^{-16}$
Chebyshev 1st Kind	$1.3834655062070259971 \times 10^{-16}$
Classical Laguerre	$8.9260826473499668326 \times 10^{-15}$
General Laguerre $\alpha = 1$	$2.4825341532472729961 \times 10^{-16}$
Hermite	$4.7043788112778503159 \times 10^{-16}$

Table 3. Newton's Method results for $n = 20$ and 30 iterations

Jacobi	Chebyshev	Gegenbauer
-0.992143445584654	-0.996917333733128	-0.991034230192877
-0.962098494639669	-0.972369920397677	-0.959770495283156
-0.90991914333223	-0.923879532511287	-0.906555627647643
-0.83679724371729	-0.852640164354092	-0.832601034386276
-0.744414638606914	-0.760405965600031	-0.739597864903566
-0.634897399553407	-0.649448048330184	-0.629673706991205
-0.510766182525352	-0.522498564715949	-0.505343420884813
-0.374878073128636	-0.382683432365090	-0.369451505240359
-0.230360787671044	-0.233445363855905	-0.22510699141448
-0.080540669675107	-0.0784590957278449	-0.0756123031135758
0.071133877871622	0.078459095727845	0.0756123031135758
0.221171767113119	0.233445363855905	0.22510699141448
0.366119581638305	0.382683432365090	0.369451505240359
0.502641066039214	0.522498564715949	0.505343420884813
0.627593920566186	0.649448048330184	0.629673706991205
0.738102136937797	0.760405965600031	0.739597864903566
0.831622222573934	0.852640164354092	0.832601034386276
0.906001841773546	0.923879532511287	0.906555627647643
0.959529848266796	0.972369920397677	0.959770495283156
0.99098031100982	0.996917333733128	0.991034230192877

Table 4. Newton's Method results for $n = 20$ and 30 iterations

Legendre	Laguerre	General Laguerre
-0.993128599185095	0.0705398896919887	0.174906752386615
-0.963971927277914	0.372126818001611	0.587303080638269
-0.912234428251326	0.916582102483273	1.23822510183424
-0.839116971822219	1.70730653102834	2.13139626007693
-0.746331906460151	2.74919925530943	3.27213313351699
-0.636053680726515	4.04892531385089	4.66749446588836
-0.510867001950827	5.61517497086162	6.32653619767384
-0.37370608871542	7.45901745367106	8.26067095201373
-0.227785851141645	9.5943928695811	10.4841673812082
-0.0765265211334974	12.0388025469643	13.0148487721526
0.0765265211334973	14.8142934426307	15.8750870127848
0.227785851141645	17.9488955205194	19.0932519076063
0.373706088715419	21.478788240285	22.7058938881731
0.510867001950827	25.4517027931869	26.7611702293794
0.636053680726515	29.9325546317006	31.3245161370075
0.746331906460151	35.013434240479	36.4887033461491
0.839116971822219	40.8330570567286	42.3934227457745
0.912234428251326	47.6199940473465	49.2688138498685
0.963971927277914	55.8107957500639	57.5544209713148
0.993128599185095	66.5244165256157	68.3770378145523

Table 5. Newton's Method results for $n = 25$ and 30 iterations

Jacobi	Chebyshev	Gegenbauer
-0.994901665878463	-0.998026728428272	-0.994174685362604
-0.975360959985654	-0.982287250728689	-0.973813483540093
-0.941256322689963	-0.951056516295154	-0.938979875687483
-0.893091307988287	-0.90482705246602	-0.890187770804335
-0.831584665110590	-0.844327925502015	-0.828161987824607
-0.757655035013272	-0.770513242775789	-0.75382448992158
-0.672406769138576	-0.684547105928689	-0.668280361715944
-0.577113343604359	-0.587785252292473	-0.57280131807384
-0.473198311079934	-0.481753674101715	-0.468806780981076
-0.362214026547642	-0.368124552684678	-0.357842771895352
-0.245818453819013	-0.248689887164855	-0.241558925568652
-0.125750396162197	-0.125333233564304	-0.121683964806954
-0.0038035200079399	8.36062906219094E-18	2.87922513006768E-17
0.118200440621912	0.125333233564304	0.121683964806954
0.238438898854630	0.248689887164855	0.241558925568652
0.355115642426439	0.368124552684678	0.357842771895352
0.466487667212620	0.481753674101715	0.468806780981076
0.570891216112889	0.587785252292473	0.57280131807384
0.666766634609609	0.684547105928689	0.668280361715944
0.752681672462637	0.770513242775789	0.75382448992158
0.827352885709386	0.844327925502015	0.828161987824607
0.889664827092574	0.904827052466020	0.890187770804335
0.938686772318027	0.951056516295154	0.938979875687483
0.973686941970036	0.982287250728689	0.973813483540093
0.994146438181037	0.998026728428272	0.994174685362604

Table 6. Newton's Method results for $n = 25$ and 30 iterations

Legendre	Laguerre	General Laguerre
-0.995556969790498	0.0567047754527055	0.141236726258096
-0.976663921459518	0.299010898586989	0.473974537884425
-0.942974571228974	0.735909555435016	0.998383405621479
-0.894991997878275	1.36918311603519	1.71638168719236
-0.833442628760834	2.20132605372147	2.63069311458477
-0.759259263037358	3.23567580355804	3.7448777262027
-0.673566368473468	4.47649661507383	5.06340831233858
-0.577662930241223	5.92908376270045	6.59177560687321
-0.473002731445715	7.59989930995675	8.33662635980513
-0.361172305809388	9.49674922093243	10.3059430256137
-0.243866883720988	11.6290149117788	12.5092780113164
-0.12286469261071	14.0079579765451	14.9580612826525
-3.94351965660777E-18	16.6471255972888	17.6660089928416
0.12286469261071	19.5628980114691	20.6496747456588
0.243866883720988	22.775241986835	23.9292078044927
0.361172305809388	26.3087723909689	27.5294209021358
0.473002731445715	30.1942911633161	31.481337894211
0.577662930241223	34.471097571922	35.8245167628475
0.673566368473468	39.1906088039374	40.61069001566
0.759259263037358	44.422349336162	45.9097868582297
0.833442628760834	50.2645749938335	51.8206158754045
0.894991997878275	56.8649671739402	58.4916748142772
0.942974571228974	64.4666706159541	66.1674493598106
0.976663921459518	73.5342347921002	75.315081358106
0.995556969790498	85.260155562496	87.1338948199813

Table 7. Newton's Method results for $n = 12$ and 30 iterations

Hermite
0.440147298645308
0.881982756213821
1.32728070207308
1.77800112433715
2.23642013026728
2.70532023717303
3.1882949244251
3.69028287699836
4.21860944438656
4.78532036735222
5.41363635528003
6.16427243405245

6. Conclusion

We have presented a unified approach for calculating the zeros of the classical orthogonal polynomials and provided examples involving the Jacobi polynomials, including Chebyshev and Gengebauer, the General Laguerre polynomials, including Legendre and Laguerre and the Hermite polynomials. We are working on a similar approach that works for more general classes of polynomials, the Heine–Stieltjes polynomials. The difficulty lies in choosing a decent guess for the zeros of the given Heine–Stieltjes polynomial. We have had some success using the electrostatic interpretation for the initial guess, but more work is needed. Other future studies include expanding the family of orthogonal polynomials to which this method applies, expanding the electrostatic interpretation to other families of polynomials, such as the generalized Bessel polynomials, and exploring connections between orthogonal polynomials and Lucas polynomial identities, such as was done in [21].

Author Contributions

All the authors equally contributed to this work. They all read and approved the final version of the paper.

Conflicts of Interest

All the authors declare no conflict of interest.

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