



## Representations for the extreme zeros of orthogonal polynomials

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### ARTICLE INFO

*Article history:*  
Received 31 August 2007

*MSC:*  
primary 42C05  
secondary 60J80

*Keywords:*  
Three-terms recurrence relation  
Interval of orthogonality  
Birth–death process  
Decay parameter

### ABSTRACT

We establish some representations for the smallest and largest zeros of orthogonal polynomials in terms of the parameters in the three-terms recurrence relation. As a corollary we obtain representations for the endpoints of the true interval of orthogonality. Implications of these results for the decay parameter of a birth–death process (with killing) are displayed.

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### 1. Introduction

This paper is concerned with representations for the smallest and largest zeros of orthogonal polynomials in terms of the parameters in the three-terms recurrence relation. Some results on the decay parameter of an ergodic birth–death process are suggestive of representations for the extreme zeros that have not yet appeared in the literature on orthogonal polynomials. Our main theorem establishes the correctness of these representations. As a corollary we obtain representations for the extreme points of the support of the orthogonalizing measure.

The paper is organized as follows. After collecting some known, but relevant properties of orthogonal polynomials in Section 2, we will derive our main results in Section 3. In Section 4 we describe some applications. In particular, we regain the results on the decay parameter of an ergodic birth–death process and extend these to the wider class of *birth–death processes with killing*.

### 2. Preliminaries

Our point of departure is the familiar three-terms recurrence relation for orthogonal polynomials. That is, we consider a sequence of monic polynomials  $\{P_n(x)\}_{n=0}^{\infty}$  satisfying

$$\begin{aligned} P_n(x) &= (x - c_n)P_{n-1}(x) - \lambda_n P_{n-2}(x), \quad n > 1, \\ P_0(x) &= 1, \quad P_1(x) = x - c_1, \end{aligned} \tag{1}$$

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where  $c_n$  is real and  $\lambda_n > 0$ . By Favard's theorem, there exists a positive Borel measure  $\psi$  on the real axis (of total mass 1, say) with respect to which the polynomials  $\{P_n(x)\}$  are orthogonal, that is,

$$\int_{-\infty}^{\infty} P_n(x)P_m(x)\psi(dx) = k_n\delta_{nm}, \quad n, m \geq 0,$$

with  $k_n > 0$ . We refer to Chihara [1] for the following preliminary results.

The polynomial  $P_n(x)$  has  $n$  real and simple zeros  $x_{n1} < x_{n2} < \dots < x_{nn}$ , and the zeros of  $P_n(x)$  and  $P_{n+1}(x)$  mutually separate each other, that is,

$$x_{n+1,i} < x_{ni} < x_{n+1,i+1}, \quad i = 1, 2, \dots, n, n \geq 1. \tag{2}$$

It follows that the limits

$$\xi_i := \lim_{n \rightarrow \infty} x_{ni} \quad \text{and} \quad \eta_i := \lim_{n \rightarrow \infty} x_{n,n-i+1}, \quad i \geq 1, \tag{3}$$

and the limits

$$\sigma := \lim_{i \rightarrow \infty} \xi_i \quad \text{and} \quad \tau := \lim_{i \rightarrow \infty} \eta_i$$

exist (but may be infinite), and satisfy

$$-\infty \leq \xi_i \leq \xi_{i+1} \leq \sigma \leq \tau \leq \eta_{i+1} \leq \eta_i \leq \infty, \quad i \geq 1. \tag{4}$$

We also recall that

$$\xi_i = \xi_{i+1} \Rightarrow \xi_j = \sigma, \quad j \geq i \quad \text{and} \quad \eta_{i+1} = \eta_i \Rightarrow \eta_j = \tau, \quad j \geq i,$$

where we use the convention  $\xi_0 := -\infty, \eta_0 := \infty$ .

Let us assume that the Hamburger moment problem associated with the polynomials  $\{P_n(x)\}$  is determined, so that  $\psi$  is the unique orthogonalizing measure for the polynomials  $\{P_n(x)\}$ . Then, if  $\xi_1 > -\infty$ , the quantities  $\xi_i$  are closely related to  $\text{supp}(\psi)$ , the support of the orthogonalizing measure  $\psi$ . Indeed, letting  $\mathcal{E} := \{\xi_1, \xi_2, \dots\}$ , we have

$$\sigma = \infty \Rightarrow \text{supp}(\psi) = \mathcal{E}, \tag{5}$$

while

$$\sigma < \infty \Rightarrow \text{supp}(\psi) \cap (-\infty, \sigma] = \bar{\mathcal{E}}, \tag{6}$$

a bar denoting closure. Moreover,  $\sigma$  is the smallest limit point of  $\text{supp}(\psi)$ . If  $\eta_1 < \infty$ , analogous statements are valid about the relation between  $\text{supp}(\psi)$  and the set  $H := \{\eta_1, \eta_2, \dots\}$ . The interpretation of  $\xi_1$  as the smallest point of  $\text{supp}(\psi)$  is relevant for the application we describe in Section 4. The interval  $[\xi_1, \eta_1]$  is sometimes referred to as the true interval of orthogonality, since there exists a unique orthogonalizing measure with support in  $[\xi_1, \eta_1]$  whether the Hamburger moment problem is determined or not.

In this paper we focus on representations for the extreme zeros  $x_{n1}$  and  $x_{nn}$ , and for the endpoints  $\xi_1$  and  $\eta_1$  of the true interval of orthogonality. We note that if  $x_{n1} < x_{n2} < \dots < x_{nn}$  are the zeros of  $P_n(x)$ , then  $-x_{nn} < -x_{n,n-1} < \dots < -x_{n1}$  are the zeros of  $P_n(-x)$ . Moreover, the polynomials  $\bar{P}_n(x) := (-1)^n P_n(-x)$  are readily seen to satisfy a recurrence relation of the type (1) with parameters  $\bar{c}_i := -c_i$  and  $\bar{\lambda}_i := \lambda_i$ . So a representation for  $x_{n1}$  (or  $\xi_1$ ) yields a representation for  $x_{nn}$  (or  $\eta_1$ ), and vice versa, simply by reversing the sign and replacing  $c_i$  by  $-c_i$ .

### 3. Representations

It will be convenient in what follows to let  $\lambda_1 := 0$ . The null vector will be denoted by  $\mathbf{0}$ , and we write  $\mathbf{a} > \mathbf{0}$  ( $\mathbf{a} \geq \mathbf{0}$ ) whenever each element of the vector  $\mathbf{a}$  is positive (nonnegative).

Denoting the  $n \times n$  identity matrix by  $I_n$ , and defining the tri-diagonal matrix

$$T_n \equiv (t_{ij}^{(n)}) := \begin{pmatrix} c_1 & \lambda_2 & 0 & \dots & 0 & 0 & 0 \\ 1 & c_2 & \lambda_3 & \dots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \dots & 1 & c_{n-1} & \lambda_n \\ 0 & 0 & 0 & \dots & 0 & 1 & c_n \end{pmatrix}, \tag{7}$$

it is easily seen that  $\det(xI_n - T_n) = P_n(x)$ , so that the zeros of  $P_n(x)$  are precisely the eigenvalues of  $T_n$ . This observation enables us to prove our main result using matrix theory.

**Theorem 1.** Let  $n > 1$ ,  $\mathbf{a} \equiv (a_1, a_2, \dots, a_n)$ , and  $a_{n+1} := 0$ . Then one has

$$x_{n1} = \max_{\mathbf{a} > \mathbf{0}} \left\{ \min_{1 \leq i \leq n} \left\{ c_i - a_{i+1} - \frac{\lambda_i}{a_i} \right\} \right\} = \min_{\mathbf{a} > \mathbf{0}} \left\{ \max_{1 \leq i \leq n} \left\{ c_i - a_{i+1} - \frac{\lambda_i}{a_i} \right\} \right\}, \tag{8}$$

and

$$x_{nn} = \min_{\mathbf{a} > \mathbf{0}} \left\{ \max_{1 \leq i \leq n} \left\{ c_i + a_{i+1} + \frac{\lambda_i}{a_i} \right\} \right\} = \max_{\mathbf{a} > \mathbf{0}} \left\{ \min_{1 \leq i \leq n} \left\{ c_i + a_{i+1} + \frac{\lambda_i}{a_i} \right\} \right\}. \tag{9}$$

**Proof.** We will prove (9). The representations for  $x_{n1}$  then follow immediately by the argument given in the last paragraph of Section 2.

Let  $c \in \mathbb{R}$  be such that  $c_i + c > 0$ , for all  $i$ ,  $1 \leq i \leq n$ . Then all elements of the matrix  $T \equiv (t_{ij}) := T_n + cI_n$  are nonnegative, so that we can apply the Perron–Frobenius theory to  $T$  (see, for example, Meyer [2, Chapter 8]). It follows in particular that  $T$  has a positive real eigenvalue equal to its spectral radius  $\rho(T)$ , and, since  $T$  is irreducible, that the corresponding left and right eigenvectors are positive. Moreover,

$$\rho(T) = \max_{\mathbf{x} > \mathbf{0}} \left\{ \min_{1 \leq i \leq n} \left\{ \frac{\sum_{j=1}^n t_{ij} x_j}{x_i} \right\} \right\} = \min_{\mathbf{x} > \mathbf{0}} \left\{ \max_{1 \leq i \leq n} \left\{ \frac{\sum_{j=1}^n t_{ij} x_j}{x_i} \right\} \right\}, \tag{10}$$

where  $\mathbf{x} \equiv (x_1, x_2, \dots, x_n)$ . Without loss of generality we can normalize  $\mathbf{x}$  such that  $x_1 = 1$ . Writing  $a_i = \lambda_i x_i / x_{i-1}$  for  $i \geq 2$  and  $a_1 = 1$ , say, the expression  $\sum_{j=1}^n t_{ij} x_j / x_i$  reduces to  $c_i + c + a_{i+1} + \lambda_i / a_i$ . Also, we must have  $\rho(T) = x_{nn} + c$ , since  $x_{ni} + c$  are the eigenvalues of  $T$ . The representations (9) are therefore implied by (10).  $\square$

**Remark.** Result (10) is known as the Collatz–Wielandt formula. The first representation in (10) can be slightly strengthened by requiring  $\mathbf{a} \geq \mathbf{0}$  only, and taking the minimum over all  $i$  such that  $a_i \neq 0$ . A similar strengthening of the second representation is not valid. (Cf. Exercises 8.2.9 and 8.2.10 in the updates on [2, Chapter 8].)

The min max representation for  $x_{nn}$  and its max min counterpart for  $x_{n1}$  were first obtained in [3] by cleverly exploiting the recurrence relation (1). The same results appeared in [4] with a proof involving Geršgorin’s circles. The other representations in Theorem 1 seem to be new. The computational benefits of the representations are clear: any choice  $\mathbf{a} > \mathbf{0}$  yields the bounds

$$\min_{1 \leq i \leq n} \{c_i - a_{i+1} - \lambda_i / a_i\} \leq x_{n1} \leq \max_{1 \leq i \leq n} \{c_i - a_{i+1} - \lambda_i / a_i\}. \tag{11}$$

We note that that by letting  $a_i = -P_{i-1}(x_{n1}) / P_{i-2}(x_{n1})$  for  $2 \leq i \leq n$  and  $a_1 = 1$ , say, we have  $\mathbf{a} > \mathbf{0}$  and

$$x_{n1} = c_i - a_{i+1} - \frac{\lambda_i}{a_i}, \quad 1 \leq i \leq n,$$

so that the two inequalities in (11) become equalities simultaneously. A similar statement obviously holds for  $x_{nn}$ . In the same vein we observe that  $\xi_1$  is the limit point of the decreasing sequence  $\{x_{n1}\}$ , so that, by choosing  $a_i = -P_{i-1}(\xi_1) / P_{i-2}(\xi_1)$  for  $i \geq 2$  and  $a_1 = 1$ , say, we have  $\mathbf{a} \equiv (a_1, a_2, \dots) > \mathbf{0}$ , and

$$\xi_1 = c_i - a_{i+1} - \lambda_i / a_i, \quad i \geq 1,$$

with a similar result being valid for  $\eta_1$ . These observations and Theorem 1 yield the following representations for the endpoints of the true interval of orthogonality.

**Corollary 2.** Let  $n > 1$  and  $\mathbf{a} \equiv (a_1, a_2, \dots)$ . Then one has

$$\xi_1 = \max_{\mathbf{a} > \mathbf{0}} \left\{ \inf_{i \geq 1} \left\{ c_i - a_{i+1} - \frac{\lambda_i}{a_i} \right\} \right\} = \min_{\mathbf{a} > \mathbf{0}} \left\{ \sup_{i \geq 1} \left\{ c_i - a_{i+1} - \frac{\lambda_i}{a_i} \right\} \right\}, \tag{12}$$

and

$$\eta_1 = \min_{\mathbf{a} > \mathbf{0}} \left\{ \sup_{i \geq 1} \left\{ c_i + a_{i+1} + \frac{\lambda_i}{a_i} \right\} \right\} = \max_{\mathbf{a} > \mathbf{0}} \left\{ \inf_{i \geq 1} \left\{ c_i + a_{i+1} + \frac{\lambda_i}{a_i} \right\} \right\}. \tag{13}$$

The max inf representation for  $\xi_1$  was first given in [5]. The other representations seem to be new.

### 4. Applications

In this section we describe an application of our results – Corollary 2 in particular – to a class of stochastic processes. But we must introduce some terminology and basic results first.

A birth–death process with killing  $\mathcal{X} \equiv \{X(t), t \geq 0\}$  is a Markov chain taking values in  $S := \{0, 1, \dots\}$  with  $q$ -matrix  $Q \equiv (q_{ij}, i, j \in S)$  given by

$$\begin{aligned} q_{i,i+1} &= \alpha_i, & q_{i+1,i} &= \beta_{i+1}, & q_{ii} &= -(\alpha_i + \beta_i + \gamma_i), \\ q_{ij} &= 0, & |i - j| &> 1, \end{aligned} \tag{14}$$

where  $\alpha_i > 0$  and  $\gamma_i \geq 0$  for  $i \geq 0$ ,  $\beta_i > 0$  for  $i > 0$ , and  $\beta_0 = 0$ . The parameters  $\alpha_i$  and  $\beta_i$  are the birth and death rates in state  $i$ , while  $\gamma_i$  may be regarded as the rate of absorption, or *killing*, into a fictitious state  $\partial$ , say. We refer to  $\mathcal{X}$  as a pure birth–death process if all killing rates are zero, with the possible exception of  $\gamma_0$ . The process  $\mathcal{X}$  is ergodic (positive recurrent) if it is a pure birth–death process satisfying  $\gamma_0 = 0$  and

$$\sum_{n=0}^{\infty} \pi_n < \infty,$$

where  $\pi_n$  are constants given by

$$\pi_0 := 1 \quad \text{and} \quad \pi_n := \frac{\alpha_0 \alpha_1 \dots \alpha_{n-1}}{\beta_1 \beta_2 \dots \beta_n}, \quad n > 0.$$

We will assume that the process  $\mathcal{X}$  is uniquely determined by its rates. (See [6] for the precise condition.)

Generalizing a classic result of Karlin and McGregor [7], we have shown in [6] (see also [8]) that the transition probabilities

$$p_{ij}(t) \equiv \Pr\{X(t) = j \mid X(0) = i\}, \quad t \geq 0, i, j \in S,$$

of the process  $\mathcal{X}$  can be represented in the form

$$p_{ij}(t) = \pi_j \int_0^{\infty} e^{-xt} R_i(x) R_j(x) \psi(dx), \quad t \geq 0, i, j \in S, \tag{15}$$

where  $R_n(x), n \geq 0$ , are polynomials defined by the recurrence relation

$$\begin{aligned} \alpha_n R_{n+1}(x) &= (\alpha_n + \beta_n + \gamma_n - x) R_n(x) - \beta_n R_{n-1}(x), & n \geq 1, \\ \alpha_0 R_1(x) &= \alpha_0 + \gamma_0 - x, & R_0(x) &= 1, \end{aligned} \tag{16}$$

and  $\psi$  is a measure of total mass 1 on the interval  $[0, \infty)$  with respect to which the polynomials  $\{R_n(x)\}$  are orthogonal. Letting

$$c_{n+1} := \alpha_n + \beta_n + \gamma_n, \quad \lambda_{n+2} := \alpha_n \beta_{n+1} \quad n \geq 0,$$

it is easily seen that the polynomials  $P_n(x) := (-1)^n \alpha_0 \alpha_1 \dots \alpha_{n-1} R_n(x), n \geq 1$ , and  $P_0(x) := R_0(x) = 1$  satisfy (1), so that we can identify the orthogonalizing measure with the measure  $\psi$  of Section 2.

The decay parameter  $\delta$  of  $\mathcal{X}$  is defined as the minimum of the exponential rates of convergence of the transition probabilities  $p_{ij}(t)$  to their limits, and may be identified with the exponential rate of convergence of  $p_{00}(t)$  to its limit (see [9–12] for proofs and developments.) A straightforward generalization of [11, Theorem 4.1] (which is formulated in terms of a pure birth–death process) expresses  $\delta$  in terms of the quantities  $\xi_i$ , namely

$$\delta = \begin{cases} \xi_2 & \text{if } \mathcal{X} \text{ is ergodic} \\ \xi_1 & \text{otherwise.} \end{cases} \tag{17}$$

Applying Corollary 2 therefore immediately yields the following.

**Theorem 3.** Let  $\alpha_{-1} := 0$  and  $\mathbf{a} \equiv (a_0, a_1, \dots)$ . The decay parameter  $\delta$  of a nonergodic (that is, transient or null recurrent) birth–death process with killing satisfies

$$\delta = \max_{\mathbf{a} > \mathbf{0}} \left\{ \inf_{i \geq 0} \left\{ \zeta_i - a_{i+1} - \frac{\alpha_{i-1} \beta_i}{a_i} \right\} \right\} = \min_{\mathbf{a} > \mathbf{0}} \left\{ \sup_{i \geq 0} \left\{ \zeta_i - a_{i+1} - \frac{\alpha_{i-1} \beta_i}{a_i} \right\} \right\}, \tag{18}$$

where  $\zeta_i \equiv \alpha_i + \beta_i + \gamma_i$ .

The max inf representation for  $\delta$  is known for pure birth–death processes (see [13] and [10]), but the min sup representation seems to be entirely new.

If  $\mathcal{X}$  is ergodic (so that, in particular,  $\gamma_i = 0$  for all  $i$ ) we can use the technique described in [9] (see also [10]) by which the calculation of  $\xi_2$  is reduced to the calculation of the smallest point in the support of an orthogonalizing measure corresponding to a dual birth–death process. Subsequently applying Corollary 2 to this dual process and translating the result in terms of the parameters of the original process  $\mathcal{X}$ , we obtain the following theorem.

**Theorem 4.** Let  $\mathbf{a} \equiv (a_0, a_1, \dots)$ . The decay parameter of an ergodic birth–death process satisfies

$$\delta = \max_{\mathbf{a} > \mathbf{0}} \left\{ \inf_{i \geq 0} \left\{ \alpha_i + \beta_{i+1} - a_{i+1} - \frac{\alpha_i \beta_i}{a_i} \right\} \right\} = \min_{\mathbf{a} > \mathbf{0}} \left\{ \sup_{i \geq 0} \left\{ \alpha_i + \beta_{i+1} - a_{i+1} - \frac{\alpha_i \beta_i}{a_i} \right\} \right\}. \quad (19)$$

The max inf representation for  $\delta$  is well known and has been proven by various techniques (see [13–15] and [10]). With the help of [14, Lemma 2.1] it can be seen that both representations in (19) are essentially given in [16, Theorem 2.3] (see also [17]). The min sup representation was observed earlier (in a finite setting) in [18] by the third author, and in [15] (see also [19]) by Granovsky and Zeifman, who established its counterpart for the other end of the spectrum in [20]. These results have inspired the research reported in this paper.

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