SANDIA REPORT

SAND2019-3362
Unlimited Release
Printed June 2018

The Basics of Orthogonal Polynomials

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Prepared by
Sandia National Laboratories
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The Basics of Orthogonal Polynomials

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Abstract

To understand the mathematics behind Uncertainty Quantification (UQ), one first needs to understand the basics of orthogonal polynomials, which this report covers.

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Definition 1 (Coefficient Sequence)**.** A coefficient sequence $\mathbf{c}$ is simply a finite sequence of complex numbers, such that, either (a) $\mathbf{c}$ is empty (*i.e.*, the sequence has no elements), or (b) $\mathbf{c}$ is non-empty and its last element is non-zero (*i.e.*, $\mathbf{c} = [c_0,\, c_1,\, c_2,\, \ldots,\, c_i]$, where $c_i \neq 0$).

Definition 2 (Polynomial)**.** Given a coefficient sequence $\mathbf{c}$, we define a function $p_{\mathbf{c}}$, that takes a complex number z as input, and returns another complex number $p_{\mathbf{c}}(z)$ as output. This function, known as the "polynomial" corresponding to the coefficient sequence $\mathbf{c}$, is given by:

$$p_{\mathbf{c}}(z) = \begin{cases} c_0 + c_1 z + c_2 z^2 + \ldots + c_i z^i = \displaystyle\sum_{j=0}^{i} c_j z^j, \text{ if } \mathbf{c} = [c_0,\, c_1,\, c_2,\, \ldots,\, c_i] \text{ is non-empty, and} \\ 0, \text{ if } \mathbf{c} \text{ is empty.} \end{cases} \tag{1}$$

Or, we could use "lambda function" notation (*e.g.*, as in Python® [1]), to say:

$$p_{\mathbf{c}} = \begin{cases} \lambda\ z : c_0 + c_1 z + c_2 z^2 + \ldots + c_i z^i = \lambda\ z : \displaystyle\sum_{j=0}^{i} c_j z^j, \text{ if } \mathbf{c} = [c_0,\, c_1,\, c_2,\, \ldots,\, c_i] \text{ is non-empty, and} \\ \lambda\ z : 0, \text{ if } \mathbf{c} \text{ is empty.} \end{cases} \tag{2}$$

Remark 3. If $\mathbf{c}$ is empty, we say that $p_{\mathbf{c}}$ is "identically zero".

Observation 4 (Canonicity of Coefficient Sequences and Polynomials)**.** If $p_{\mathbf{c_1}}$ and $p_{\mathbf{c_2}}$ are identical polynomial functions (*i.e.*, $p_{\mathbf{c_1}}(z) = p_{\mathbf{c_2}}(z)$, for every complex number z), then their corresponding coefficient sequences, $\mathbf{c_1}$ and $\mathbf{c_2}$, must be identical as well. Conversely, if two coefficient sequences $\mathbf{c_1}$ and $\mathbf{c_2}$ are identical, then their corresponding polynomial functions, $p_{\mathbf{c_1}}$ and $p_{\mathbf{c_2}}$, will also be identical (by Definition 2).

Definition 5 (Degree of a Polynomial)**.** Given a polynomial $p_{\mathbf{c}}$, corresponding to the coefficient sequence $\mathbf{c}$, we define the degree of $p_{\mathbf{c}}$ as follows:

$$\text{degree}\,(p_{\mathbf{c}}) = \begin{cases} i, \text{ if } \mathbf{c} = [c_0,\, c_1,\, c_2,\, \ldots,\, c_i] \text{ is non-empty, and} \\ -1, \text{ if } \mathbf{c} \text{ is empty.} \end{cases} \tag{3}$$

Definition 6 (Monic Polynomial)**.** A polynomial $p_{\mathbf{c}}$, corresponding to the coefficient sequence $\mathbf{c}$, is called "monic" if (a) $\mathbf{c}$ is non-empty, and (b) the highest coefficient $c_i = 1$ (where $\mathbf{c} = [c_0,\, c_1,\, c_2,\, \ldots,\, c_i]$).

Remark 7. We denote the set of complex numbers by $\mathbb{C}$, the set of real numbers by $\mathbb{R}$, and the set of integers by $\mathbb{Z}$.

Definition 8 (Real Polynomial)**.** A polynomial $p_{\mathbf{c}}$, corresponding to the coefficient sequence $\mathbf{c}$, is called "real" if either, (a) $\mathbf{c}$ is empty, or (b) (if $\mathbf{c}$ is non-empty) the coefficients in $\mathbf{c}$ are all real; that is, $c_j \in \mathbb{R}$ for every integer j such that $0 \leq j \leq i$ (where $\mathbf{c} = [c_0,\, c_1,\, c_2,\, \ldots,\, c_i]$).

Definition 9 (Moment Functional)**.** Given an infinite sequence of complex numbers $\mu = [\mu_0,\, \mu_1,\, \mu_2,\, \ldots]$, we define a function $\mathcal{L}_\mu$, that takes a polynomial $p_{\mathbf{c}}$ as input, and returns a complex number $\mathcal{L}_\mu(p_{\mathbf{c}})$

as output. This function, known as the "moment functional" associated with the "moment sequence" μ, is given by:

$$\mathcal{L}_\mu(p_{\mathbf{c}}) = \begin{cases} \mathcal{L}_\mu\left(\lambda\, z : \sum_{j=0}^{i} c_j z^j\right) = \sum_{j=0}^{i} c_j\, \mu_j, \text{ if } \mathbf{c} = [c_0,\, c_1,\, c_2,\, \ldots,\, c_i] \text{ is non-empty, and} \\ 0, \text{ if } \mathbf{c} \text{ is empty.} \end{cases} \tag{4}$$

Observation 10. With the above definition, we have $\mathcal{L}_\mu\big(\lambda\, z : z^i\big) = \mu_i$, for every integer $i \geq 0$.

Observation 11. $\mathcal{L}_\mu$ is "additive". That is,

$$\mathcal{L}_\mu(p_{\mathbf{c_1}} + p_{\mathbf{c_2}}) = \mathcal{L}_\mu(\lambda\, z : p_{\mathbf{c_1}}(z) + p_{\mathbf{c_2}}(z)) = \mathcal{L}_\mu(p_{\mathbf{c_1}}) + \mathcal{L}_\mu(p_{\mathbf{c_2}}) \text{, for any two polynomials } p_{\mathbf{c_1}} \text{ and } p_{\mathbf{c_2}}. \tag{5}$$

Observation 12. $\mathcal{L}_\mu$ is "homogeneous". That is,

$$\mathcal{L}_\mu(\alpha\, p_{\mathbf{c}}) = \mathcal{L}_\mu(\lambda\, z : \alpha\, p_{\mathbf{c}}(z)) = \alpha\, \mathcal{L}_\mu(p_{\mathbf{c}}) \text{, for any polynomial } p_{\mathbf{c}} \text{ and any complex number } \alpha. \tag{6}$$

Observation 13. $\mathcal{L}_\mu$ is "linear", because it satisfies the additivity and homogeneity conditions above.

Example 14 (Weighted Integral Moment Functional)**.** This moment functional will be of particular interest to us. Given a non-negative "weight function" w, with a positive measure, that is defined on the real interval $[a,\, b]$, we define the corresponding moment sequence $\mu = \{\mu_i \mid i \in \mathbb{Z},\, i \geq 0\}$ to be:

$$\mu_i = \int_{x=a}^{b} w(x)\, x^i\, dx \tag{7}$$

In particular, we will be interested in the case where the weight function w above happens to be the probability density function of a random variable.

Definition 15 (Orthogonal Polynomial Sequence or OPS)**.** Given a moment functional $\mathcal{L}_\mu$, we define an infinite sequence of polynomials $\mathbf{p}_{\mathcal{L}_\mu} = [p_{\mathbf{c_0}},\, p_{\mathbf{c_1}},\, p_{\mathbf{c_2}},\, \ldots]$ (corresponding to the coefficient sequences $[\mathbf{c_0},\, \mathbf{c_1},\, \mathbf{c_2},\, \ldots]$ respectively) to be an orthogonal polynomial sequence (or OPS) with respect to $\mathcal{L}_\mu$, if the following three conditions are satisfied:

1. For every integer $i \geq 0$, $p_{\mathbf{c_i}}$ is a polynomial of degree i,
2. For every two integers i and j such that $i \geq 0$, $j \geq 0$, and $i \neq j$, we have:

$$\mathcal{L}_\mu\big(p_{\mathbf{c_i}} \times p_{\mathbf{c_j}}\big) = \mathcal{L}_\mu\big(\lambda\, z : p_{\mathbf{c_i}}(z) \times p_{\mathbf{c_j}}(z)\big) = 0, \text{ and} \tag{8}$$

3. For every integer $i \geq 0$, we have:

$$\mathcal{L}_\mu\big(p_{\mathbf{c_i}}^2\big) = \mathcal{L}_\mu(\lambda\, z : p_{\mathbf{c_i}}(z) \times p_{\mathbf{c_i}}(z)) \neq 0. \tag{9}$$

Observation 16. Given an arbitrary moment sequence μ, there may or may not exist an OPS associated with $\mathcal{L}_\mu$.

Observation 17. Let $\mathbf{p}_{\mathcal{L}_\mu} = [p_{\mathbf{c_0}},\, p_{\mathbf{c_1}},\, p_{\mathbf{c_2}},\, \ldots]$ be an OPS, with respect to the moment functional $\mathcal{L}_\mu$. Then, $\mathbf{q}_{\mathcal{L}_\mu} = [\beta_0\, p_{\mathbf{c_0}},\, \beta_1\, p_{\mathbf{c_1}},\, \beta_2\, p_{\mathbf{c_2}},\, \ldots]$ is also an OPS with respect to $\mathcal{L}_\mu$, for any sequence of non-zero complex numbers $[\beta_0,\, \beta_1,\, \beta_2,\, \ldots]$. Thus, if an OPS with respect to $\mathcal{L}_\mu$ exists, then there exist infinitely many OPSes with respect to $\mathcal{L}_\mu$.

Definition 18 (Monic OPS)**.** An OPS $\mathbf{p}_{\mathcal{L}_\mu} = [p_{\mathbf{c_0}},\, p_{\mathbf{c_1}},\, p_{\mathbf{c_2}},\, \ldots]$ is called "monic" if every polynomial $(p_{\mathbf{c_0}}, p_{\mathbf{c_1}}, p_{\mathbf{c_2}}, \ldots)$ in the OPS is monic (as in Definition 6).

Definition 19 ($\mathbf{K}$-OPS)**.** Given (a) a moment functional $\mathcal{L}_\mu$, and (b) an infinite sequence of non-zero complex numbers, $\mathbf{K} = [K_0,\, K_1,\, K_2,\, \ldots]$, we define $\mathbf{p}_{\mathcal{L}_\mu} = [p_{\mathbf{c_0}},\, p_{\mathbf{c_1}},\, p_{\mathbf{c_2}},\, \ldots]$ to be a $\mathbf{K}$-OPS with respect to $\mathcal{L}_\mu$, if it is an OPS with respect to $\mathcal{L}_\mu$ that, in addition to satisfying the regular OPS conditions of Definition 15, also satisfies the following:

$$\mathcal{L}_\mu\big(z^i\, p_{\mathbf{c_i}}\big) = \mathcal{L}_\mu\big(\lambda\, z : z^i \times p_{\mathbf{c_i}}(z)\big) = K_i, \text{ for every integer } i \geq 0. \tag{10}$$

Definition 20 (Normalised OPS, or Orthonormal Polynomial Sequence)**.** Given a moment functional $\mathcal{L}_\mu$, we define $\mathbf{p}_{\mathcal{L}_\mu} = [p_{\mathbf{c_0}},\, p_{\mathbf{c_1}},\, p_{\mathbf{c_2}},\, \ldots]$ to be a "normalised" OPS with respect to $\mathcal{L}_\mu$, or an orthonormal polynomial sequence with respect to $\mathcal{L}_\mu$, if it is an OPS with respect to $\mathcal{L}_\mu$ that, in addition to satisfying the regular OPS conditions of Definition 15, also satisfies the following:

$$\mathcal{L}_\mu\big(p_{\mathbf{c_i}}^2\big) = 1, \text{ for every integer } i \geq 0. \tag{11}$$

Definition 21 (Positively Oriented Complex Number)**.** We say that a complex number $z = \text{Re}(z) + \sqrt{-1}.\text{Im}(z)$ is "positively oriented" if it lies either in the open right half of the complex plane, or on the positive imaginary axis. That is, we have:

$$(\text{Re}(z) > 0) \text{ or } (\text{Re}(z) = 0 \text{ and } \text{Im}(z) > 0) \tag{12}$$

Definition 22 (Positively Oriented OPS)**.** Given a moment functional $\mathcal{L}_\mu$, we define $\mathbf{p}_{\mathcal{L}_\mu} = [p_{\mathbf{c_0}},\, p_{\mathbf{c_1}},\, p_{\mathbf{c_2}},\, \ldots]$ to be a "positively oriented" OPS with respect to $\mathcal{L}_\mu$ if it is an OPS with respect to $\mathcal{L}_\mu$ that, in addition to satisfying the regular OPS conditions of Definition 15, is also such that, for each $i \geq 0$, the highest coefficient in $p_{\mathbf{c_i}}$ (*i.e.*, the coefficient of z^i in the expansion of $p_{\mathbf{c_i}}(z)$) is positively oriented.

Definition 23 (Negatively Oriented OPS)**.** Given a moment functional $\mathcal{L}_\mu$, we define $\mathbf{p}_{\mathcal{L}_\mu} = [p_{\mathbf{c_0}},\, p_{\mathbf{c_1}},\, p_{\mathbf{c_2}},\, \ldots]$ to be a "negatively oriented" OPS with respect to $\mathcal{L}_\mu$ if it is an OPS with respect to $\mathcal{L}_\mu$ that, in addition to satisfying the regular OPS conditions of Definition 15, is also such that, for each $i \geq 0$, the highest coefficient in $p_{\mathbf{c_i}}$ (*i.e.*, the coefficient of z^i in the expansion of $p_{\mathbf{c_i}}(z)$) lies in the region of the complex plane given by $\{z \,|\, \text{Re}(z) < 0 \text{ or } (\text{Re}(z) = 0 \text{ and } \text{Im}(z) < 0)\}$ (*i.e.*, the open left half of the complex plane, plus the negative imaginary axis).

Observation 24. An OPS may be neither positively nor negatively oriented.

Theorem 25. *Let $\mathbf{p}_{\mathcal{L}_\mu} = [p_{\mathbf{c_0}},\, p_{\mathbf{c_1}},\, p_{\mathbf{c_2}},\, \ldots]$ be an OPS, with respect to the moment functional $\mathcal{L}_\mu$. Then, $p_{\mathbf{c_0}} = \lambda\, z : c$, where c is a non-zero complex number.*

Proof. From the first condition of Definition 15, $p_{\mathbf{c_0}}$ is a polynomial of degree 0. That is, we have:

$$\text{degree}\,(p_{\mathbf{c_0}}) = 0. \tag{13}$$

From Definition 5, this is possible only when the coefficient sequence $\mathbf{c_0}$ has exactly one element. This element, from Definition 1, must be a complex number. If we call this complex number c, we have:

$$\mathbf{c_0} = [c]. \tag{14}$$

Applying Definition 2 to the above, we have:

$$p_{\mathbf{c_0}} = \lambda\, z : c. \tag{15}$$

Now, all that's left to prove is that $c \neq 0$. This we can see from Definition 1: c, being the last element of a non-empty coefficient sequence $\mathbf{c_0}$, has to be non-zero. ☐

Theorem 26. *Let $\mathbf{p}_{\mathcal{L}_\mu} = [p_{\mathbf{c_0}}, p_{\mathbf{c_1}}, p_{\mathbf{c_2}}, \ldots]$ be an OPS, with respect to the moment functional $\mathcal{L}_\mu$. Then, for every $i \geq 1$, $\mathcal{L}_\mu(p_{\mathbf{c_i}}) = 0$.*

Proof. From Theorem 25, let $p_{\mathbf{c_0}} = \lambda\, z : c$, where c is a non-zero complex number. Then, for every $i \geq 1$, we have:

$$\begin{aligned}
\mathcal{L}_\mu(p_{\mathbf{c_i}}) &= \frac{c}{c}\,\mathcal{L}_\mu(p_{\mathbf{c_i}}) \\
&= \frac{1}{c}\,\mathcal{L}_\mu(c\,p_{\mathbf{c_i}}) && \text{(from Observation 12)} \\
&= \frac{1}{c}\,\mathcal{L}_\mu(p_{\mathbf{c_0}} \times p_{\mathbf{c_i}}) \\
&= \frac{1}{c}\,0 && \text{(from the second condition of Definition 15)} \\
&= 0.
\end{aligned} \tag{16}$$

☐

Definition 27 (Vector Spaces of Polynomials)**.** For every $i \geq 0$, we define $\mathbb{P}_i$ to be the vector space of polynomials of degree at most i, over the field of complex numbers $\mathbb{C}$. Operations such as field addition, field multiplication, vector addition, and multiplication of a vector by a scalar, are assumed to be done "the natural way" and are not defined precisely here.

Observation 28. For every $i \geq 0$, the set of polynomials given by $\{\lambda\, z : z^j \mid 0 \leq j \leq i\}$ forms a basis for the vector space $\mathbb{P}_i$. Thus, the dimension of $\mathbb{P}_i$ is $i + 1$ [2].

Theorem 29 (Basis Sets of Orthogonal Polynomials)**.** *Let $\mathbf{p}_{\mathcal{L}_\mu} = [p_{\mathbf{c_0}}, p_{\mathbf{c_1}}, p_{\mathbf{c_2}}, \ldots]$ be an OPS, with respect to the moment functional $\mathcal{L}_\mu$. Then, for every $i \geq 0$, the set of polynomials $\{p_{\mathbf{c_0}}, p_{\mathbf{c_1}}, p_{\mathbf{c_2}}, \ldots, p_{\mathbf{c_i}}\}$ forms a basis for the vector space $\mathbb{P}_i$.*

Proof. For every $i \geq 1$, because $p_{\mathbf{c_i}}$ is of degree i, it cannot be written as a linear combination of the polynomials $\{p_{\mathbf{c_0}}, p_{\mathbf{c_1}}, p_{\mathbf{c_2}}, \ldots, p_{\mathbf{c_{i-1}}}\}$, which all have smaller degrees. Therefore, the polynomials $\{p_{\mathbf{c_0}}, p_{\mathbf{c_1}}, p_{\mathbf{c_2}}, \ldots, p_{\mathbf{c_i}}\}$ are linearly independent. But these are $i+1$ linearly independent "vectors" from the vector space $\mathbb{P}_i$, which, by Observation 28, is of dimension $i+1$. Therefore, by the dimension theorem for vector spaces (see, for example, [2]), the polynomials $\{p_{\mathbf{c_0}}, p_{\mathbf{c_1}}, p_{\mathbf{c_2}}, \ldots, p_{\mathbf{c_i}}\}$ must form a basis for $\mathbb{P}_i$. ☐

Theorem 30. *Let $\mathbf{p}_{\mathcal{L}_\mu} = [p_{\mathbf{c_0}}, p_{\mathbf{c_1}}, p_{\mathbf{c_2}}, \ldots]$ be an OPS, with respect to the moment functional $\mathcal{L}_\mu$. Then, for each $i \geq 0$, $\mathcal{L}_\mu(q \times p_{\mathbf{c_i}}) = 0$ for every polynomial q of degree smaller than i, and $\mathcal{L}_\mu(q \times p_{\mathbf{c_i}}) \neq 0$ for every polynomial q of degree equal to i.*

Proof. Let q be a polynomial of degree j, which is at most i.

Now, if q is identically zero (*i.e.*, $j = -1$), then $q \times p_{\mathbf{c_i}}$ will also be identically zero for every $i \geq 0$, and thus $\mathcal{L}_\mu(q \times p_{\mathbf{c_i}})$ will trivially be zero (from Definition 9) for every $i \geq 0$. So let us just consider situations where $j \geq 0$. That is,

$$\text{degree}\,(q) = j, \text{ where } 0 \leq j \leq i. \tag{17}$$

Then, by the "basis sets of orthogonal polynomials" theorem (Theorem 29), we can write q as a linear combination of the polynomials in $\{p_{\mathbf{c_0}}, p_{\mathbf{c_1}}, p_{\mathbf{c_2}}, \ldots, p_{\mathbf{c_j}}\}$. That is, we have:

$$q = \sum_{k=0}^{j} \alpha_k \; p_{\mathbf{c_k}} \tag{18}$$

Also, in the expansion above, the last coefficient α_j will be non-zero. This is because the left hand side (q) of the equation above is of degree j, and if α_j were zero, the linear combination on the right hand side would have a degree strictly smaller than j, which would be a contradiction. Thus, we have:

$$\alpha_j \neq 0. \tag{19}$$

Multiplying Eq. (18) by $p_{\mathbf{c_i}}$ and applying $\mathcal{L}_\mu$ to both sides, we get:

$$\begin{aligned}
\mathcal{L}_\mu(q \times p_{\mathbf{c_i}}) &= \mathcal{L}_\mu\left(\left(\sum_{k=0}^{j} \alpha_k \; p_{\mathbf{c_k}}\right) \times p_{\mathbf{c_i}}\right) \\
&= \mathcal{L}_\mu\left(\sum_{k=0}^{j} \alpha_k \; (p_{\mathbf{c_k}} \times p_{\mathbf{c_i}})\right) \\
&= \sum_{k=0}^{j} \alpha_k \; \mathcal{L}_\mu(p_{\mathbf{c_k}} \times p_{\mathbf{c_i}}) \qquad \text{(by the linearity of } \mathcal{L}_\mu, \textit{ i.e.}, \text{ Observation 13)}
\end{aligned} \tag{20}$$

Now, from Eq. (17), $j \leq i$. If $j < i$, each term in the summation above vanishes due to the second condition from Definition 15. But if $j = i$, the last term in the summation (corresponding to

$k = j = i$) alone survives. Thus, we have:

$$\mathcal{L}_\mu(q \times p_{\mathbf{c_i}}) = \begin{cases} 0, \text{ if } j < i, \text{ and} \\ \alpha_i \, \mathcal{L}_\mu\big(p^2_{\mathbf{c_i}}\big), \text{ if } j = i. \end{cases} \tag{21}$$

But if $j = i$, we have $\alpha_i \neq 0$ from Eq. (19), and we also have $\mathcal{L}_\mu\big(p^2_{\mathbf{c_i}}\big) \neq 0$ from the third condition of Definition 15. Therefore, Eq. (21) allows us to conclude that, for every $i \geq 0$:

$$\mathcal{L}_\mu(q \times p_{\mathbf{c_i}}) \begin{cases} = 0, \text{ if degree}\,(q) < i, \text{ and} \\ \neq 0, \text{ if degree}\,(q) = i, \end{cases} \tag{22}$$

where we have replaced j by degree$\,(q)$ using Eq. (17). □

Theorem 31 (Converse of Theorem 30)**.** *Let* $\mathbf{p} = [p_{\mathbf{c_0}}, p_{\mathbf{c_1}}, p_{\mathbf{c_2}}, \ldots]$ *be an infinite sequence of polynomials (with coefficient sequences* $[\mathbf{c_0}, \mathbf{c_1}, \mathbf{c_2}, \ldots]$ *respectively), where* $p_{\mathbf{c_i}}$ *has degree* i*, for every* $i \geq 0$*. Also, let* $\mathcal{L}_\mu$ *be a moment functional, with respect to the moment sequence* $[\mu_0, \mu_1, \mu_2, \ldots]$*. Suppose that, for every* $i \geq 0$*, we have* $\mathcal{L}_\mu(q \times p_{\mathbf{c_i}}) = 0$ *for every polynomial* q *of degree smaller than* i*, and that* $\mathcal{L}_\mu(q \times p_{\mathbf{c_i}}) \neq 0$ *for every polynomial* q *of degree equal to* i*. Then,* $\mathbf{p}$ *is an OPS with respect to* $\mathcal{L}_\mu$*.*

Proof. Since, for every $i \geq 0$, $p_{\mathbf{c_i}}$ is given to be a polynomial of degree i, the sequence $\mathbf{p}$ clearly satisfies the first condition of Definition 15. Now, choose any $i > 0$ and $j > 0$. There are only three possibilities:

1. $i < j$. In this case, letting "q" $= p_{\mathbf{c_i}}$ and "i" $= j$ in "$\mathcal{L}_\mu(q \times p_{\mathbf{c_i}}) = 0$ for every polynomial q of degree smaller than i", we get $\mathcal{L}_\mu\big(p_{\mathbf{c_i}} \times p_{\mathbf{c_j}}\big) = 0$.
2. $i > j$. In this case, letting "q" $= p_{\mathbf{c_j}}$ and "i" $= i$ in "$\mathcal{L}_\mu(q \times p_{\mathbf{c_i}}) = 0$ for every polynomial q of degree smaller than i", we get $\mathcal{L}_\mu\big(p_{\mathbf{c_j}} \times p_{\mathbf{c_i}}\big) = \mathcal{L}_\mu\big(p_{\mathbf{c_i}} \times p_{\mathbf{c_j}}\big) = 0$.
3. $i = j$. In this case, letting "q" $= p_{\mathbf{c_i}}$ and "i" $= j \; (= i)$ in "$\mathcal{L}_\mu(q \times p_{\mathbf{c_i}}) \neq 0$ for every polynomial q of degree equal to i", we get $\mathcal{L}_\mu\big(p_{\mathbf{c_i}} \times p_{\mathbf{c_j}}\big) = \mathcal{L}_\mu\big(p^2_{\mathbf{c_i}}\big) \neq 0$.

Thus, we have:

$$\mathcal{L}_\mu\big(p_{\mathbf{c_i}} \times p_{\mathbf{c_j}}\big) \begin{cases} = 0, \text{ if } i \neq j, \text{ and} \\ = \mathcal{L}_\mu\big(p^2_{\mathbf{c_i}}\big) \neq 0, \text{ if } i = j, \end{cases} \tag{23}$$

which shows that the sequence $\mathbf{p}$ satisfies the second and third conditions of Definition 15. Therefore, $\mathbf{p}$ is an OPS with respect to $\mathcal{L}_\mu$. □

Theorem 32. *Let* $\mathbf{p}_{\mathcal{L}_\mu} = [p_{\mathbf{c_0}}, p_{\mathbf{c_1}}, p_{\mathbf{c_2}}, \ldots]$ *be an OPS, with respect to the moment functional* $\mathcal{L}_\mu$*. Then, for every* $i \geq 0$*, given any polynomial* q *of degree* i*, we can write* q *as:*

$$q = \sum_{j=0}^{i} \alpha_j \, p_{\mathbf{c_j}},$$

$$\text{where } \alpha_j = \frac{\mathcal{L}_\mu\big(q \times p_{\mathbf{c_j}}\big)}{\mathcal{L}_\mu\Big(p^2_{\mathbf{c_j}}\Big)}, \text{ for every } 0 \leq j \leq i. \tag{24}$$

Proof. From Theorem 29, we already know that the set of polynomials $\{p_{\mathbf{c_0}},\, p_{\mathbf{c_1}},\, p_{\mathbf{c_2}},\, \ldots,\, p_{\mathbf{c_i}}\}$ forms a basis for the vector space $\mathbb{P}_i$, for every $i \geq 0$. Also, q, being a polynomial of degree i, is a member of the vector space $\mathbb{P}_i$. Therefore, q can be written as a linear combination of the polynomials $\{p_{\mathbf{c_0}},\, p_{\mathbf{c_1}},\, p_{\mathbf{c_2}},\, \ldots,\, p_{\mathbf{c_i}}\}$. That is, we have:

$$q = \sum_{j=0}^{i} \alpha_j \, p_{\mathbf{c_j}} \tag{25}$$

Multiplying both sides of the above equation by $p_{\mathbf{c_k}}$ (where $0 \leq k \leq i$), and applying $\mathcal{L}_\mu$ to both sides, we get:

$$\begin{aligned}
\mathcal{L}_\mu(q \times p_{\mathbf{c_k}}) &= \mathcal{L}_\mu\left(\left(\sum_{j=0}^{i} \alpha_j \, p_{\mathbf{c_j}}\right) \times p_{\mathbf{c_k}}\right) \\
&= \mathcal{L}_\mu\left(\sum_{j=0}^{i} \alpha_j \,(p_{\mathbf{c_j}} \times p_{\mathbf{c_k}})\right) \\
&= \sum_{j=0}^{i} \alpha_j \, \mathcal{L}_\mu\big(p_{\mathbf{c_j}} \times p_{\mathbf{c_k}}\big) \qquad \text{(by the linearity of } \mathcal{L}_\mu, \textit{ i.e.}, \text{ Observation 13)}
\end{aligned} \tag{26}$$

From the second condition in Definition 15, we see that only the term corresponding to $j = k$ survives in the summation above; the rest of the terms vanish. Therefore, we have:

$$\mathcal{L}_\mu(q \times p_{\mathbf{c_k}}) = \alpha_k \, \mathcal{L}_\mu(p_{\mathbf{c_k}} \times p_{\mathbf{c_k}}) = \alpha_k \, \mathcal{L}_\mu\big(p_{\mathbf{c_k}}^2\big)\,, \text{ for every } k \in \{0,\, 1,\, 2,\, \ldots,\, i\} \tag{27}$$

Dividing both sides by $\mathcal{L}_\mu\big(p_{\mathbf{c_k}}^2\big)$ (which we know to be non-zero from the third condition of Definition 15) we get:

$$\alpha_k = \frac{\mathcal{L}_\mu(q \times p_{\mathbf{c_k}})}{\mathcal{L}_\mu\big(p_{\mathbf{c_k}}^2\big)}, \text{ for every } k \in \{0,\, 1,\, 2,\, \ldots,\, i\} \tag{28}$$

Changing the dummy index variable from k to j in Eq. (28), we get:

$$\alpha_j = \frac{\mathcal{L}_\mu\big(q \times p_{\mathbf{c_j}}\big)}{\mathcal{L}_\mu\Big(p_{\mathbf{c_j}}^2\Big)}, \text{ for every } j \in \{0,\, 1,\, 2,\, \ldots,\, i\} \tag{29}$$

Combining Eq. (25) and Eq. (29), we get:

$$\begin{aligned}
&q = \sum_{j=0}^{i} \alpha_j \, p_{\mathbf{c_j}} \\
&\text{where } \alpha_j = \frac{\mathcal{L}_\mu\big(q \times p_{\mathbf{c_j}}\big)}{\mathcal{L}_\mu\Big(p_{\mathbf{c_j}}^2\Big)}, \text{ for every } 0 \leq j \leq i.
\end{aligned} \tag{30}$$

□

Theorem 33 (Uniqueness of OPS upto constant factors)**.** *Given a moment functional $\mathcal{L}_\mu$. Let $\mathbf{p} = [p_{\mathbf{c_0}}, p_{\mathbf{c_1}}, p_{\mathbf{c_2}}, \ldots]$ and $\mathbf{q} = [q_{\mathbf{d_0}}, q_{\mathbf{d_1}}, q_{\mathbf{d_2}}, \ldots]$ be two orthogonal polynomial sequences associated with $\mathcal{L}_\mu$, with coefficient sequences $[\mathbf{c_0}, \mathbf{c_1}, \mathbf{c_2}, \ldots]$ and $[\mathbf{d_0}, \mathbf{d_1}, \mathbf{d_2}, \ldots]$ respectively. Then, the polynomials in $\mathbf{p}$ and those in $\mathbf{q}$ will only differ by constant factors; that is, for every $i \geq 0$, $q_{\mathbf{d_i}} = \beta_i \, p_{\mathbf{c_i}}$, where $[\beta_0, \beta_1, \beta_2, \ldots]$ is a sequence of non-zero complex numbers.*

Proof. Applying Theorem 32, we can write the polynomial $q_{\mathbf{d_i}}$ (which is of degree i) as a linear combination of the polynomials $\{p_{\mathbf{c_0}}, p_{\mathbf{c_1}}, p_{\mathbf{c_2}}, \ldots, p_{\mathbf{c_i}}\}$, as follows:

$$q_{\mathbf{d_i}} = \sum_{j=0}^{i} \alpha_j \, p_{\mathbf{c_j}},$$
$$\text{where } \alpha_j = \frac{\mathcal{L}_\mu\big(q_{\mathbf{d_i}} \times p_{\mathbf{c_j}}\big)}{\mathcal{L}_\mu\Big(p_{\mathbf{c_j}}^2\Big)}. \tag{31}$$

But applying Theorem 30, with $q_{\mathbf{d}}$ as the sequence of orthogonal polynomials, $q_{\mathbf{d_i}}$ as the i^{th} polynomial (with degree i) in the sequence, and $p_{\mathbf{c_j}}$ (for $0 \leq j \leq i$) as the “arbitrary” polynomial of degree at most i, we get:

$$\mathcal{L}_\mu\big(p_{\mathbf{c_j}} \times q_{\mathbf{d_i}}\big) = \mathcal{L}_\mu\big(q_{\mathbf{d_i}} \times p_{\mathbf{c_j}}\big) \begin{cases} = 0, & \text{if } i < j, \text{ and} \\ \neq 0, & \text{if } i = j, \end{cases} \tag{32}$$

for every j from 0 to i.

From Eq. (31) and Eq. (32), we see that only the last term (corresponding to $j = i$) in the summation on the right hand side of Eq. (31) survives; the rest of the terms vanish because $\alpha_j = 0$ for every j from 0 to $i - 1$. Therefore, we have:

$$q_{\mathbf{d_i}} = \underbrace{\frac{\mathcal{L}_\mu(q_{\mathbf{d_i}} \times p_{\mathbf{c_i}})}{\mathcal{L}_\mu(p_{\mathbf{c_i}}^2)}}_{\beta_i} \, p_{\mathbf{c_i}}, \text{ for every } i \geq 0. \tag{33}$$

The complex numbers β_i in the equation above are all non-zero. We know this because each β_i is a fraction, where we know the numerator to be non-zero from the “$i = j$” case of Eq. (32), and the denominator to be non-zero from the third condition of Definition 15. ☐

Remark 34. Theorem 33 tells us that, given a moment functional $\mathcal{L}_\mu$, orthogonal polynomial sequences with respect to $\mathcal{L}_\mu$ are essentially unique — except for the non-zero constant factors β_i above.

But often, for concreteness, we will need to single out a particular OPS for discussion, without having to worry about these constant factors. In such cases, we will typically follow one of the three approaches below:

1. We will insist that the OPS be monic (as in Definition 18), or

2. We will specify an infinite sequence of non-zero complex numbers, $\mathbf{K} = [K_0, K_1, K_2, \ldots]$, and we will insist that the OPS be a $\mathbf{K}$-OPS with respect to $\mathcal{L}_\mu$ (as in Definition 19), or
3. We will insist (a) that the OPS be normalised (as in Definition 20), and (b) that the OPS be either positively (as in Definition 22) or negatively (as in Definition 23) oriented.

Each of the above is enough to guarantee uniqueness. For example, given a moment functional $\mathcal{L}_\mu$, if there exists an OPS for it, there will also exist a monic OPS for it, and this monic OPS will be unique (see Theorem 35). Similarly, given a moment functional $\mathcal{L}_\mu$, if there exists an OPS for it, there will also exist a unique $\mathbf{K}$-OPS for it, with respect to any sequence of non-zero complex numbers $\mathbf{K}$ (see Theorem 36). And finally, given a moment functional $\mathcal{L}_\mu$, if there exists an OPS for it, there will also exist a unique positively/negatively oriented, normalised OPS for it (see Theorem 37).

Moreover, given a moment functional $\mathcal{L}_\mu$, and any OPS for it, it is easy to get from it the corresponding monic OPS, or the corresponding $\mathbf{K}$-OPS with respect to any sequence of non-zero complex numbers $\mathbf{K}$, or the corresponding positively/negatively oriented, normalised OPS.

We state the following theorems without proof.

Theorem 35. *Given a moment functional $\mathcal{L}_\mu$, such that an OPS with respect to $\mathcal{L}_\mu$ exists. Then, there exists a unique monic OPS with respect to $\mathcal{L}_\mu$.*

Theorem 36. *Given (a) a moment functional $\mathcal{L}_\mu$, such that an OPS with respect to $\mathcal{L}_\mu$ exists, and (b) an infinite sequence of non-zero complex numbers, $\mathbf{K} = [K_0, K_1, K_2, \ldots]$. Then, there exists a unique $\mathbf{K}$-OPS with respect to $\mathcal{L}_\mu$.*

Theorem 37. *Given a moment functional $\mathcal{L}_\mu$, such that an OPS with respect to $\mathcal{L}_\mu$ exists. Then, there exists a unique positively oriented, normalised OPS with respect to $\mathcal{L}_\mu$, and a unique negatively oriented, normalised OPS with respect to $\mathcal{L}_\mu$.*

Definition 38 (Moment Matrices)**.** Given a moment sequence $\mu = [\mu_0, \mu_1, \mu_2, \ldots]$, we define an infinite sequence of square matrices, $\mathbf{M}_\mu = \left[\mathbf{M}_{(0,\mu)}, \mathbf{M}_{(1,\mu)}, \mathbf{M}_{(2,\mu)}, \ldots\right]$, known as "moment matrices", as follows:

$$\mathbf{M}_{(i,\mu)} = \begin{bmatrix} \mu_0 & \mu_1 & \mu_2 & \cdots & \mu_i \\ \mu_1 & \mu_2 & \mu_3 & \cdots & \mu_{i+1} \\ \mu_2 & \mu_3 & \mu_4 & \cdots & \mu_{i+2} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \mu_i & \mu_{i+1} & \mu_{i+2} & \cdots & \mu_{2i} \end{bmatrix}, \text{ for every } i \geq 0. \tag{34}$$

Definition 39 (Moment Determinants)**.** Given a moment sequence $\mu = [\mu_0, \mu_1, \mu_2, \ldots]$, we define an infinite sequence of complex numbers, $\mathbf{d}_\mu = \left[d_{(0,\mu)}, d_{(1,\mu)}, d_{(2,\mu)}, \ldots\right]$, known as "moment determinants", as follows:

$$d_{(i,\mu)} = \det\left(\mathbf{M}_{(i,\mu)}\right) = \begin{vmatrix} \mu_0 & \mu_1 & \mu_2 & \cdots & \mu_i \\ \mu_1 & \mu_2 & \mu_3 & \cdots & \mu_{i+1} \\ \mu_2 & \mu_3 & \mu_4 & \cdots & \mu_{i+2} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \mu_i & \mu_{i+1} & \mu_{i+2} & \cdots & \mu_{2i} \end{vmatrix}, \text{ for every } i \geq 0. \tag{35}$$

Theorem 40 (Existence of OPS)**.** *Let $\mathcal{L}_\mu$ be a moment functional, corresponding to the moment sequence $\mu = [\mu_0, \mu_1, \mu_2, \ldots]$. Then, a necessary and sufficient condition for the existence of an OPS with respect to $\mathcal{L}_\mu$ is that the moment matrices $\left[\mathbf{M}_{(0,\mu)}, \mathbf{M}_{(1,\mu)}, \mathbf{M}_{(2,\mu)}, \ldots\right]$ (as defined in Definition 38) are all non-singular, i.e., the moment determinants $\left[d_{(0,\mu)}, d_{(1,\mu)}, d_{(2,\mu)}, \ldots\right]$ (as defined in Definition 39) are all non-zero.*

Theorem 41. *Given (a) a moment functional $\mathcal{L}_\mu$, and (b) a $\mathbf{K}$-OPS $\mathbf{p}_{\mathcal{L}_\mu} = [p_{\mathbf{c_0}}, p_{\mathbf{c_1}}, p_{\mathbf{c_2}}, \ldots]$ with respect to $\mathcal{L}_\mu$, corresponding to the sequence $\mathbf{K} = [K_0, K_1, K_2, \ldots]$ (as in Definition 19). Then, for every $i \geq 0$, the highest coefficient $c_{(i,i)}$ of $p_{\mathbf{c_i}}$, i.e., the last element of $\mathbf{c_i}$, or the coefficient multiplying z^i in the expansion of $p_{\mathbf{c_i}}(z)$, is given by:*

$$c_{(i,i)} = \frac{K_i \, d_{(i-1,\mu)}}{d_{(i,\mu)}}, \tag{36}$$

where $d_{(-1,\mu)}$ is defined to be 1.

Definition 42 ($\mathbf{S}$-positive definiteness)**.** Given an infinite set of real numbers $\mathbf{S}$, a moment functional $\mathcal{L}_\mu$ is called "positive definite with respect to $\mathbf{S}$", or "$\mathbf{S}$-positive definite", if, for every polynomial p that is (a) non-negative on $\mathbf{S}$ (*i.e.*, $p(x) \geq 0$ for every $x \in \mathbf{S}$), and (b) not identically zero, we have $\mathcal{L}_\mu(p) > 0$.

Definition 43 (Positive definiteness)**.** A moment functional $\mathcal{L}_\mu$ is called "positive definite" if it is $\mathbf{S}$-positive definite, when $\mathbf{S} = (-\infty, \infty)$.

Theorem 44 ($\mathbf{S}$-positive definiteness implies positive definiteness)**.** *Let $\mathcal{L}_\mu$ be an $\mathbf{S}$-positive definite moment functional, with respect to the infinite set $\mathbf{S}$. Then, $\mathcal{L}_\mu$ is also positive definite.*

Theorem 45. *Let $\mathcal{L}_\mu$ be a positive definite moment functional, corresponding to the moment sequence $\mu = [\mu_0, \mu_1, \mu_2, \ldots]$. Then, for every $i \geq 0$, μ_i is real and $\mu_{2i} > 0$.*

Theorem 46. *Let $\mathcal{L}_\mu$ be a positive definite moment functional. Then, an OPS with respect to $\mathcal{L}_\mu$ exists.*

Theorem 47. *Let p be a polynomial that is non-negative on $(-\infty, \infty)$, i.e., $p(x) \geq 0$ for all real x. Then, p can always be written as the sum of squares of two real polynomials. That is, we have:*

$$p = q^2 + r^2, \tag{37}$$

where q and r are real polynomials (as in Definition 8).

Theorem 48. *Let $\mathcal{L}_\mu$ be a moment functional, corresponding to the moment sequence $\mu = [\mu_0, \mu_1, \mu_2, \ldots]$. Then, $\mathcal{L}_\mu$ is positive definite if and only if (a) μ_i is real for every $i \geq 0$, and (b) $d_{(i,\mu)} > 0$ for every $i \geq 0$.*

Theorem 49. *Let $\mathbf{p}_{\mathcal{L}_\mu} = [p_{\mathbf{c_0}}, p_{\mathbf{c_1}}, p_{\mathbf{c_2}}, \ldots]$ be an OPS, with respect to the moment functional $\mathcal{L}_\mu$. Then, if (a) $p_{\mathbf{c_i}}$ is real for every $i \geq 0$, and (b) $\mathcal{L}_\mu(p^2_{\mathbf{c_i}}) > 0$ for every $i \geq 0$, then $\mathcal{L}_\mu$ is positive definite.*

Theorem 50 (Three-term Recurrence Formula)**.** *Let $\mathbf{p}_{\mathcal{L}_\mu} = [p_{\mathbf{c_0}}, p_{\mathbf{c_1}}, p_{\mathbf{c_2}}, \ldots]$ be an OPS, with respect to the moment functional $\mathcal{L}_\mu$. Then, there exist three sequences of complex numbers, $\gamma = [\gamma_1, \gamma_2, \gamma_3, \ldots]$, $\delta = [\delta_1, \delta_2, \delta_3, \ldots]$, and $\theta = [\theta_2, \theta_3, \theta_4, \ldots]$, such that, for every $z \in \mathbb{C}$, we have:*

$$p_{\mathbf{c_1}}(z) = \left(\frac{z - \delta_1}{\gamma_1}\right) p_{\mathbf{c_0}}(z)\,, \text{ and}$$

$$p_{\mathbf{c_i}}(z) = \left(\frac{z-\delta_i}{\gamma_i}\right)\, p_{\mathbf{c_{i-1}}}(z) - \left(\frac{\theta_i}{\gamma_i}\right)\, p_{\mathbf{c_{i-2}}}(z)\,, \text{ for every } i \geq 2. \tag{38}$$

In particular, we have:

$$\begin{aligned}
\gamma_i &= \frac{\mathcal{L}_\mu\big(z\, p_{\mathbf{c_{i-1}}}\, p_{\mathbf{c_i}}\big)}{\mathcal{L}_\mu\big(p^2_{\mathbf{c_i}}\big)}, \text{ for every } i \geq 1, \\
\delta_i &= \frac{\mathcal{L}_\mu\Big(z\, p^2_{\mathbf{c_{i-1}}}\Big)}{\mathcal{L}_\mu\Big(p^2_{\mathbf{c_{i-1}}}\Big)}, \text{ for every } i \geq 1, \text{ and} \\
\theta_i &= \frac{\mathcal{L}_\mu\big(z\, p_{\mathbf{c_{i-2}}}\, p_{\mathbf{c_{i-1}}}\big)}{\mathcal{L}_\mu\Big(p^2_{\mathbf{c_{i-2}}}\Big)}, \text{ for every } i \geq 2.
\end{aligned} \tag{39}$$

References

[1] https://docs.python.org/3/tutorial/controlflow.html#lambda-expressions.

[2] https://en.wikipedia.org/wiki/Dimension_theorem_for_vector_spaces.

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