Spectral Theory of Orthogonal Polynomials

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Lecture 1: Introduction and Overview
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- Lecture 2: Szegö Theorem for OPUC
- Lecture 3: Three Kinds of Polynomials Asymptotics, I
- Lecture 4: Three Kinds of Polynomial Asymptotics, II
References


Spectral theory is the general theory of the relation of the fundamental parameters of an object and its “spectral” characteristics.

Spectral characteristics means eigenvalues or scattering data or, more generally, spectral measures.
What is spectral theory

Examples include

- Can you hear the shape of a drum?
- Computer tomography
- Isospectral manifold for the harmonic oscillator
What is spectral theory?

The *direct problem* goes from the object to spectra.

The *inverse problem* goes backwards.

The direct problem is typically easy while the inverse problem is typically hard.

For example, the domain of definition of the harmonic oscillator isospectral “manifold” is unknown. It is not even known if it is connected!
Orthogonal polynomials on the real line (OPRL) and on the unit circle (OPUC) are particularly useful because the inverse problems are easy—indeed the inverse problem is the OP definition as we’ll see.

OPs also enter in many application—both specific polynomials and the general theory.
Indeed, my own interest came from studying discrete Schrödinger operators on $\ell^2(\mathbb{Z})$

$$(Hu)_n = u_{n+1} + u_{n-1} + V u_n$$

and the realization that when restricted to $\mathbb{Z}_+$, one had a special case of OPRL.
μ will be a probability measure on \( \mathbb{R} \). We’ll always suppose that \( \mu \) has bounded support \([a, b]\) which is not a finite set of points. (We then say that \( \mu \) is non-trivial.) This implies that \( 1, x, x^2, \ldots \) are independent since
\[
\int |P(x)|^2 \, d\mu = 0 \Rightarrow \mu \text{ is supported on the zeroes of } P.
\]

Apply Gram Schmidt to \( 1, x, \ldots \) and get monic polynomials
\[
P_j(x) = x^j + \alpha_{j,1}x^{j-1} + \ldots
\]

and orthonormal (ON) polynomials
\[
p_j = P_j/\|P_j\|
\]
More generally we can do the same for any probability measure of bounded support on $\mathbb{C}$.

One difference from the case of $\mathbb{R}$, the linear combination of $\{x^j\}_{j=0}^{\infty}$ are dense in $L^2(\mathbb{R}, d\mu)$ by Weierstrass. This may or may not be true if $\text{supp}(d\mu) \not\subset \mathbb{R}$.

If $d\mu = d\theta/2\pi$ on $\partial \mathbb{D}$, the span of $\{z^j\}_{j=0}^{\infty}$ is not dense in $L^2$ (but is only $H^2$). Perhaps, surprisingly, we’ll see later that there are measures $d\mu$ on $\partial \mathbb{D}$ for which they are dense (e.g., $\mu$ purely singular).

More significantly, the argument we’ll give for our recursion relation fails if $\text{supp}(d\mu) \not\subset \mathbb{R}$. 
Since $P_k$ is monic and $\{P_j\}_{j=0}^{k+1}$ span polynomials of degree at most $k+1$, we have

$$xP_k = P_{k+1} + \sum_{j=0}^{k} B_{k,j} P_j$$

Clearly

$$B_{k,j} = \frac{\langle P_j, xP_k \rangle}{\|P_j\|^2}$$

Now we use

$$\langle P_j, xP_k \rangle = \langle xP_j, P_k \rangle$$

(need $d\mu$ on $\mathbb{R}$!!)

If $j < k - 1$, this is zero.

If $j = k - 1$, $\langle P_{k-1}, xP_k \rangle = \langle xP_{k-1}, P_k \rangle = \|P_k\|^2$. 

(need $d\mu$ on $\mathbb{R}$!!)
Thus \((P_{-1} \equiv 0)\); \(\{a_j\}_{j=1}^{\infty}, \{b_j\}_{j=1}^{\infty}\) : Jacobi recursion

\[ xP_N = P_{N+1} + b_{N+1}P_N + a_N^2P_{N-1} \]

\[ b_N \in \mathbb{R}, \quad a_N = \|P_N\|/\|P_{N-1}\| \]

These are called Jacobi parameters. This implies
\[ \|P_N\| = a_N a_{N-1} \ldots a_1 \text{ (since } \|P_0\| = 1). \]

This, in turn, implies \(p_n = P_n/a_1 \ldots a_n\) obeys

\[ xp_n = a_{n+1}p_{n+1} + b_{n+1}p_n + a_np_{n-1} \]
We have thus solved the inverse problem, i.e., $\mu$ is the spectral data and $\{a_n, b_n\}_{n=1}^\infty$ are the descriptors of the object.

In the orthonormal basis $\{p_n\}_{n=0}^\infty$, multiplication by $x$ has the matrix

$$J = 
\begin{pmatrix}
b_1 & a_1 & 0 & 0 & \ldots \\
a_1 & b_2 & a_2 & 0 & \ldots \\
0 & a_2 & b_3 & a_3 & \ldots \\
\vdots & \vdots & \vdots & \vdots & \ddots
\end{pmatrix}
$$

called a Jacobi matrix.
Favard’s Theorem

Since

\[ b_n = \int x p_{n-1}^2(x) \, d\mu, \quad a_n = \int x p_{n-1}(x) p_n(x) \, d\mu \]

\( \text{supp}(\mu) \subset [-R, R] \Rightarrow |b_n| \leq R, \ |a_n| \leq R. \)

Conversely, if \( \sup_n (|a_n| + |b_n|) = \alpha < \infty \), \( J \) is a bounded matrix of norm at most \( 3\alpha \). In that case, the spectral theorem implies there is a measure \( d\mu \) so that

\[ \langle (1, 0, \ldots)^t, J^\ell (1, 0, \ldots)^t \rangle = \int x^\ell \, d\mu(x) \]

If one uses Gram-Schmidt to orthonormalize \( \{J^\ell (1, 0, \ldots)^t\}_{\ell=0}^\infty \), one finds \( \mu \) has Jacobi matrix exactly given by \( J \).
We have thus proven Favard’s Theorem (his paper was in 1935; really due to Stieltjes in 1894 or to Stone in 1932).

**Favard’s Theorem.** There is a one-one correspondence between bounded Jacobi parameters

\[ \{a_n, b_n\}_{n=1}^{\infty} \in \left(0, \infty \right) \times \mathbb{R} \]

and non-trivial probability measures, \( \mu \), of bounded support via:

\[ \mu \Rightarrow \{a_n, b_n\} \quad (\text{OP recursion}) \]

\[ \{a_n, b_n\} \Rightarrow \mu \quad (\text{Spectral Theorem}) \]

There are also results for \( \mu \)'s with unbounded support so long as \( \int x^n \, d\mu < \infty \). In this case, \( \{a_n, b_n\} \Rightarrow \mu \) may not be unique because \( J \) may not be essentially self-adjoint on vectors of finite support.
Let $d\mu$ be a non-trivial probability measure on $\partial \mathbb{D}$. As in the OPRL case, we use Gram-Schmidt to define monic OPs, $\Phi_n(t)$ and ON OP’s $\varphi_n(z)$.

In the OPRL case, if $z$ is multiplication by the underlying variable, $z^* = z$. This is replaced by $z^*z = 1$.

In the OPRL case, $P_{n+1} - xP_n \perp \{1, x_1, \ldots, x_{n-2}\}$. 
In the OPUC case, $\Phi_{n+1} - z\Phi_n \perp \{z, \ldots, z^n\}$, since
\[
\langle z\Phi, z^j \rangle = \langle \Phi, z^{j-1} \rangle
\]
if $j \geq 1$.

In the OPRL case, we used $\deg P = n$ and $P \perp \{1, x, \ldots, x^{n-2}\} \Rightarrow P = c_1 P_n + c_2 P_{n-1}$.

In the OPUC case, we want to characterize $\deg P = n$, $P \perp \{z, z^2, \ldots, z^n\}$. 
Define $*$ on degree $n$ polynomials to themselves by

$$Q^*(z) = z^n Q\left(\frac{1}{\bar{z}}\right)$$

(bad but standard notation!) or

$$Q(z) = \sum_{j=0}^{n} c_j z^j \Rightarrow Q^*(z) = \sum_{j=0}^{n} \bar{c}_{n-j} z^j$$

Then, $*$ is unitary and so for deg $Q = n$

$$Q \perp \{1, \ldots, z^{n-1}\} \iff Q = c \Phi_n$$

is equivalent to

$$Q \perp \{z, \ldots, z^n\} \iff Q = c \Phi_n^*$$
Szegő recursion and Verblunsky coefficients

Thus, we see, there are parameters \( \{\alpha_n\}_{n=0}^{\infty} \) (called Verblunsky coefficients) so that

\[
\Phi_{n+1}(z) = z\Phi_n - \bar{\alpha}_n \Phi^*_n(z)
\]

This is the Szegő Recursion (History: Szegő and Geronimus in 1939; Verblunsky in 1935–36)

Applying * for deg \( n + 1 \) polynomials to this yields

\[
\Phi^*_{n+1}(z) = \Phi^*_n(z) - \alpha_n z\Phi_n
\]

The strange looking \(-\bar{\alpha}_n\) rather than say \(+\alpha_n\) is to have the \( \alpha_n \) be the Schur parameter of the Schur function of \( \mu \) (Geronimus); also the Verblunsky parameterization then agrees with \( \alpha_n \). These are discussed in [OPUC1].
$\Phi_n$ monic $\Rightarrow$ constant term in $\Phi^*_n$ is 1 $\Rightarrow$ $\Phi^*_n(0) = 1$.

This plus $\Phi_{n+1} = z\Phi_n - \bar{\alpha}_n \Phi^*_n(z)$ implies

$$-\Phi_{n+1}(0) = \alpha_n$$

i.e., $\Phi_n$ determines $\alpha_{n-1}$. 
Szegő recursion and Verblunsky coefficients

For OPRL, we saw $\|P_{n+1}\|/\|P_n\| = a_{n+1}$. We are looking for the analog for OPUC.

Szegő Recursion $\Rightarrow \Phi_{n+1} + \bar{\alpha}_n \Phi_n^* = z \Phi_n$

$$\Phi_{n+1} \perp \Phi_n^* \Rightarrow \|\Phi_{n+1}\|^2 + |\alpha_n|^2 \|\Phi_n\|^2 = \|z \Phi_n\|^2$$

Multiplication by $z$ unitary plus $^*$ antiunitary $\Rightarrow$

$$\|\Phi_{n+1}\|^2 = \rho_n^2 \|\Phi_n\|^2; \quad \rho_n^2 = 1 - |\alpha_n|^2$$

which implies $|\alpha_n| < 1$ (i.e., $\alpha_n \in \mathbb{D}$) and

$$\|\Phi_n\| = \rho_{n-1} \cdots \rho_0$$
Szegő recursion and Verblunsky coefficients

\[
\begin{pmatrix}
\varphi_{n+1} \\
\varphi_n^*
\end{pmatrix}
= A_n(z)
\begin{pmatrix}
\varphi_n \\
\varphi_n^*
\end{pmatrix}
x; \\
A_n = \rho_n^{-1}
\begin{pmatrix}
z & -\bar{\alpha}_n \\
-\alpha_n z & 1
\end{pmatrix}
\]

\[\det A_n \neq 0 \text{ if } z \neq 0, \text{ so we can get } \varphi_n (\Phi_n) \text{ from } \varphi_{n+1} (\Phi_{n+1}) \text{ by} \]

\[
z\Phi_n = \rho_n^{-2}\left[\Phi_{n+1} + \bar{\alpha}_n \Phi_{n+1}^*\right]
\]

\[
\Phi_n^* = \rho_n^{-2}\left[\Phi_{n+1} + \alpha_n \Phi_{n+1}\right]
\]
Szegő recursion and Verblunsky coefficients

We see that \( \Phi_{n+1} \) determines \( \alpha_n \), so by induction and inverse recursion,

**Theorem.** If two measures have the same \( \Phi_n \), they have the same \( \{ \Phi_j \}_{j=0}^n \) and \( \{ \alpha_j \}_{j=0}^{n-1} \).
Szegő recursion and Verblunsky coefficients

A similar argument to the one that led to $|\alpha_n| < 1$ yields

**Theorem.** All zeros of $\Phi_n$ lie in $\mathbb{D}$.

**Proof.** $\Phi_n(z_0) = 0 \Rightarrow \Phi_n = (z - z_0)p$, $\deg p = n - 1$

$zp = \Phi_n + z_0p$ and $p \perp \Phi_n \Rightarrow \|p\|^2 = \|\Phi_n\|^2 + |z_0|^2 \|p\|^2$

$\Rightarrow |z_0| < 1$

**Corollary.** All zeros of $\Phi_n^*(z)$ lie in $\mathbb{C} \setminus \overline{\mathbb{D}}$. 
Here is a second proof that only uses Szegő recursion. By induction, suppose that all zeros of $\Phi_n$ are in $\mathbb{D}$. Then, for $|\beta| < 1$

$$z\Phi_n + \beta\Phi_n^* \neq 0 \text{ on } \partial\mathbb{D}$$

since $|z\Phi_n(z)| = |\Phi_n^*(z)|$ on $\partial\mathbb{D}$. ($\frac{1}{\bar{z}} = z$)

If $\Phi^{(\beta)}_{n+1} = z\Phi_n + \beta\Phi_n^*$, then at $\beta = 0$, all zeros of $\Phi^{(\beta)}_{n+1}$ are in $\mathbb{D}$.

As $\beta$ varies in $\mathbb{D}$, all zeros of $\Phi^{(\beta)}_{n+1}$ are trapped in $\mathbb{D}$. QED.
Bernstein–Szegő Approximation

We are heading towards a proof that any \( \{ \alpha_n \}_{n=0}^{\infty} \subset \mathbb{D} \) are the Verblunsky coefficients of a measure on \( \partial \mathbb{D} \) (analog of Favard’s Theorem). It will depend on

**Theorem** (Bernstein–Szegő measures). Let
\[
\{ \alpha_j^{(0)} \}_{j=0}^{n-1} \subset \mathbb{D}^n.
\]
Let \( \varphi_n(z) \) be the normalized degree \( n \) polynomial obtained by Szegő recursion. Let
\[
d\mu_n(\theta) = \frac{d\theta}{2\pi|\varphi_n(z)|^2}
\]

Then \( d\mu_n \) has Verblunsky coefficients
\[
\alpha_j(d\mu_n) = \begin{cases} 
\alpha_j^{(0)} & j = 0, \ldots, n - 1 \\
0 & j \geq n
\end{cases}
\]
The first step of the proof is to show that

\[ k, \ell, n \text{ with } k < n + \ell \Rightarrow \int_{z=e^{i\theta}} \bar{z}^k z^\ell \varphi_n(z) d\mu_n(\theta) = 0 \]

For \( z \in \partial \mathbb{D} \Rightarrow \varphi_n(z) = \overline{\varphi_n\left(\frac{1}{\bar{z}}\right)} = z^{-n} \varphi_n^*(z). \)

Thus the integral above is

\[
\int \frac{\bar{z}^k z^\ell \varphi_n(z)}{z^{-n} \varphi_n(z) \varphi_n^*(z)} \frac{dz}{2\pi i z} = \frac{1}{2\pi} \int \frac{\varphi_n^*(z)}{\varphi_n^*(z)} = \frac{1}{2\pi} \int \frac{dz}{z^{\ell+n-k-1} \varphi_n^*(z)}
\]

is zero since \( \left[ \varphi_n^*(z) \right]^{-1} \) is analytic on a neighborhood of \( \overline{\mathbb{D}} \) and \( \ell + n - k - 1 \geq 0. \)
Thus, $z^\ell \varphi_n$ is a multiple of the OP’s for $d\mu_n$.

Since $\int |z^\ell \varphi_n|^2 d\mu = 1$, we see that

$$\varphi_{n+k}(z; d\mu) = z^k \varphi_n(z); \ k > 0.$$  

As we saw, $\Phi_n$ determines $\{\alpha_j\}_{j=0}^{n-1}$ and $\Phi_j$ by inverse Szegő recursion and $-\Phi_{j+1}(0) = \alpha_j$. This shows that

$$\varphi_j(z; d\mu) = \begin{cases} \varphi_j(x) & j = 0, \ldots, n \\ z^{j-n} \varphi_n(z) & j = n, n + 1, \ldots \end{cases}$$

implying the claimed result.
Bernstein–Szegő Approximation

Given \( \{\alpha_j\}_{j=0}^{\infty} \subset \mathbb{D} \), we can form \( d\mu_n \) as above via
\[
\int \Phi_j(e^{i\theta}) d\mu(e^{i\theta}) = 0, \quad \{\Phi_j\}_{j=0}^{n} \text{ determines } \{\int z^j d\mu\}_{j=0}^{n}
\]
inductively (actually they determine more moments). Thus
\[
\int z^j d\mu_n = \int z^j d\mu_m \quad j \leq \min(n, m)
\]
and
\[
\int \overline{z}^j d\mu_n = (\int z^j d\mu_n).
\]
Thus, \( d\mu_n \) has a weak limit \( d\mu_\infty \). Clearly, \( \alpha_j(d\mu_\infty) = \alpha_j \).

We have thus proven

**Verblunsky’s Theorem.** \( \mu \rightarrow \{\alpha_j(\mu)\}_{j=0}^{\infty} \) sets up a 1–1 correspondence between non-trivial probability measures on \( \partial \mathbb{D} \) and \( \mathbb{D}^{\infty} \).
Carmona Simon Formula

Simon [CRM Proc. and Lecture Notes 42 (2007), 453–463] has proven an analog of the Bernstein–Szegő approximation for OPRL (the analog for Schrödinger operators is due to Carmona; hence the name):

Let $d\rho$ be a probability measure on $\mathbb{R}$ with $\int|x|^n\,d\rho < \infty$ for all $n$. Let $\{p_n\}_{n=0}^{\infty}$ be its orthonormal polynomials and $\{a_n, b_n\}_{n=1}^{\infty}$ its Jacobi parameters. Let

$$d\nu_n(x) = \frac{dx}{\pi(a_n^2p_n^2(x) + p_{n-1}^2(x))}$$

Then, for $\ell = 0, \ldots, 2n - 2$, $\int x^\ell \,d\nu_n = \int x^\ell \,d\rho$.

If the moment problem for $d\rho$ is determinate, then $d\nu_n \rightarrow d\rho$ weakly.
One important consequence of this result is

**Theorem.** If $I \subset \mathbb{R}$ is an interval and for all $x \in I$ and some $c > 0$, we have that

$$c \leq a_n^2 p_n^2(x) + p_{n-1}^2(x) \leq c^{-1}$$

then $d\rho \upharpoonright I$ has a.c. part and no singular spectrum.

Similarly, for $I \subset \partial \mathbb{D}$ and $\mu$ a probability measure

$$c \leq |\varphi_n(z)| \leq c^{-1} \quad \text{all } z \in I$$

implies $d\mu \upharpoonright I$ has a.c. part and no singular spectrum.

**Remark.** A much stronger result is known (see e.g., Simon [Proc AMS 124 (1996), 3361]); $I$ can be any set and $c$ can be $x$-dependent.