Mecánica Cuántica y Entropías de Polinomios Ortogonales

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Motivation I

WHY? To study the internal disorder of quantum systems.

HOW? By means of

- Quantum Physics
- Information Theory

QUANTUM PHYSICS

- Schrödinger formulation: Wave Mechanics
  Quantum states → Wavefunctions → Special Functions (O.P.’s)
  Equation of motion: Schrödinger equation

- Heisenberg formulation: Matrix Mechanics
  Quantum states → $N \times 1$ matrices
  Dynamical variables satisfy a matricial equation of motion
  Usually, matrices are hermitian $N \times N$ matrices
Motivation II

INFORMATION THEORY

- Spreading measures of wavefunctions: Information-theoretic measures of orthogonal polynomials.
  - The variance

\[ V[\rho] = \langle x^2 \rangle - \langle x \rangle^2 = \int_{\Delta} x^2 \rho(x) dx - \left( \int_{\Delta} x \rho(x) dx \right)^2 \]

- The Fisher information

\[ F[\rho] = \langle \left( \frac{d}{dx} \log \rho(x) \right)^2 \rangle = \int_{\Delta} \frac{[\rho'(x)]^2}{\rho(x)} dx \]

- The Shannon entropy

\[ S[\rho] = -\langle \log \rho(x) \rangle = -\int_{\Delta} \rho(x) \log \rho(x) dx \]

Notation: \( \langle f(x) \rangle := \int_{\Delta} f(x) \rho(x) dx \)

- New kind of entropies: the entropy of a matrix
Wave Mechanics
and
Continuous Entropy of Orthogonal Polynomials
Schrödinger equation I

\[
\left[-\frac{1}{2}\nabla^2 + V(r)\right] \psi (\vec{r}, t) = i\hbar \frac{\partial}{\partial t} \psi (\vec{r}, t)
\]

Quantum states. Wavefunctions

\[
\psi_{nlm} (\vec{r}, t) = \psi_{nlm}(\vec{r}) \exp (\frac{-i E_{nlm} t}{\hbar}),
\]

\[
\begin{align*}
n & = 1, 2, ... \\
l & = 0, 1, 2, ..., n - 1 \\
m & = -l, -l + 1, ..., l
\end{align*}
\]

where \( \{E, \psi_{nlm}(\vec{r})\} \) are the eigensolutions of the Hamiltonian.
Schrödinger equation II

For central potentials

\[ \psi_{nlm}(\vec{r}) = R_{nl}(r) Y_{lm}(\theta, \phi) \]

with

\[ R_{nl}(r) = \begin{cases} y_n(r) \sqrt{\omega_l} & \text{Orthogonal function of h.p. type} \\ \text{or} \\ \text{any other special function of A.M} \end{cases} \]

and

\[ Y_{lm}(\theta, \phi) \quad \text{are the spherical harmonics} \]
Spherical harmonics and Gegenbauer polynomials

\[ Y_{lm}(\theta, \phi) = \frac{1}{\sqrt{2\pi}} C_{l-m}^{l+m} (\cos \theta) (\sin \theta)^m e^{im\phi} \]

with \(0 \leq \theta \leq \pi\) and \(0 \leq \phi \leq 2\pi\) and \(C_n^\lambda(x)\) are polynomials orthogonal with respect to the weight function

\[ \omega_\lambda(x) = (1 - x^2)^{\lambda-1/2}; \quad -1 \leq x \leq 1 \]

so that

\[ \int_{-1}^{1} C_n^\lambda(x) C_m^\lambda(x) \omega(x) dx = \frac{\pi 2^{1-2\lambda} \Gamma(n + 2\lambda)}{n!(n + \lambda)\Gamma^2(\lambda)} \delta_{nm} \]
Schrödinger equation IV

**Quantum-mechanical probability in** \((\vec{r}, \vec{r} + d\vec{r})\)

\[
\rho_{nlm}(\vec{r}) d\vec{r} = |\Psi_{nlm}(\vec{r}, t)|^2 d\vec{r} = |\psi_{nlm}(\vec{r})|^2 r^2 dr d\Omega \\
= |R_{nl}(\vec{r})|^2 r^2 dr \times |Y_{lm}(\theta, \phi)|^2 d\Omega \\
\equiv D_{nl}(r) r^2 dr \times \Pi_{lm}(\Omega) d\Omega
\]

(i) the radial probability density

\[
D_{nl}(r) = |R_{nl}(r)|^2 = [y_n(r)]^2 \omega_l(r)
\]

gives the probability per radial interval to find the particle in \((r, r + dr)\),
the angular probability density

\[ \Pi_{lm}(\Omega) = |Y_{lm}(\theta, \phi)|^2 = \left[ C_{l+m}^{l-m}(\cos \theta) \right]^2 [\sin \theta]^{2m} \]

describes the spatial profile of the system

Comments:

- The internal disorder of the system can be measured by means of the **spreading measures of** \( D_{nl}(r) \), which are power (variance), derivative (Fisher information) or logarithmic (Shannon entropy) functionals of the involved orthogonal polynomials.

- The system profile can be estimated by means of the **spreading measures of** \( \Pi_{lm}(\Omega) \), which are given by the corresponding functionals of the Gegenbauer polynomials.
Rakhmanov density of some special functions

- For orthogonal polynomials $y_n(x)$:
  \[
  \rho_n(x) = [y_n(x)]^2 \omega(x)
  \]

- For spherical harmonics $Y_{lm}(\theta, \phi)$
  \[
  \rho_{lm}(\theta, \phi) = |Y_{lm}(\theta, \phi)|^2
  \]
Rakhmanov density of the Jacobi polynomials $P_{n}^{(\alpha,\beta)}(x)$

- Rakhmanov-Jacobi densities for $\alpha = 2$ and $\beta = 3$

\[
\rho_n(x) = \left[ P_n^{(2,3)}(x) \right]^2 (1 - x)^2 (1 + x)^3; \quad -1 \leq x \leq +1
\]
Rakhmanov density of the Laguerre polynomials $L_n^{(\alpha)}(x)$

- Rakhmanov-Laguerre densities for $\alpha = 2$

$$\rho_n(x) = \left[ L_n^{(2)}(x) \right]^2 x^2 e^{-x}; \quad 0 \leq x < +\infty$$
Rakhmanov density of the Hermite polynomials $H_n(x)$

- Rakhmanov-Hermite densities

$$\rho_n(x) = [H_n(x)]^2 e^{-x^2}; \quad -\infty < x < +\infty$$
Rakhmanov density of spherical harmonics $Y_{lm}(\theta, \phi)$

- Spherical harmonics with $l = 3$ and $m = 0$

$$|Y_{3,0}(\theta, \phi)|^2$$
Rakhmanov density of spherical harmonics $Y_{lm}(\theta, \phi)$ II

- Spherical harmonics with $l = 3$ and $m = 1$

$|Y_{3,1}(\theta, \phi)|^2$
Rakhmanov density of spherical harmonics $Y_{lm}(\theta, \phi)$ III

- Spherical harmonics with $l = 3$ and $m = 2$

\[ |Y_{3,2}(\theta, \phi)|^2 \]
Spherical harmonics with $l = 3$ and $m = 3$

$$|Y_{3,3}(\theta, \phi)|^2$$
Spreading measures for central potentials and orthogonal polynomials

Quantum-mechanical density

\[ \rho_{nlm}(\vec{r}) = D_{nl}(r) \times \Pi_{lm}(\theta, \phi) \]

with the Rakhmanov densities

\[ D_{nl}(r) = [y_n(r)]^2 \omega_l(r) \quad \text{and} \quad \Pi_{lm}(\theta, \phi) = |Y_{lm}(\theta, \phi)|^2 \]
Heisenberg measure (Variance)

\[ V[\rho_{nlm}] := \langle r^2 \rangle - \langle r \rangle^2 \]

\[ = \int_0^\infty r^4 [y_n(r)]^2 \omega_l(r) \, dr - \left| \int_0^\infty r^3 [y_n(r)]^2 \omega_l(r) \, dr \right|^2 \]
**Fisher information**

\[
F[\rho_{nlm}] := \int_{\mathbb{R}^3} \left| \nabla \rho_{nlm}(\vec{r}) \right|^2 \rho_{nlm}(\vec{r}) d\vec{r} = 4 \int_{\mathbb{R}^3} \left| \nabla^{1/2} \rho_{nlm}(\vec{r}) \right|^2 d\vec{r} = F(D_{nl}) + \langle r^{-2} \rangle F(\Pi_{lm})
\]

where

\[
\langle r^{-2} \rangle = \int_0^\infty [y_n(r)]^2 \omega_l(r) dr \equiv N_{nl}
\]

is the norm of the polynomials involved in the wavefunction. Here

\[
F(D_{nl}) = 4 \int_0^\infty \left\{ \frac{d}{dr} \left[ y_n(r) \sqrt{\omega_l(r)} \right] \right\}^2 r^2 dr
\]

and

\[
F(\Pi_{lm}) = 4 \int_\Omega \left| \frac{d}{d\theta} Y_{lm}(\theta, 0) \right|^2 d\Omega
\]

are the radial and angular parts, respectively.
Spreading measures for central potentials and O.P. III

**Shannon entropy**

\[
S \left[ \rho_{nlm} \right] := - \int_{\mathbb{R}^3} \rho_{nlm}(\vec{r}) \log \left[ \rho_{nlm}(\vec{r}) \right] d\vec{r} = S(D_{nl}) + S(\Pi_{lm})
\]

where

\[
S(D_{nl}) = - \int_{0}^{\infty} D_{nl}(r) \log \left[ D_{nl}(r) \right] dr
\]

\[
= - \int_{0}^{\infty} \omega_l(r) y_n^2(r) \log \left[ \omega_l(r) y_n^2(r) \right] dr \equiv E[y_n]
\]

and

\[
S(\Pi_{lm}) = - \int_{\Omega} \Pi_{lm}(\Omega) \log \left[ \Pi_{lm}(\Omega) \right] d\Omega
\]

\[
= - \int_{0}^{\pi} \sin \theta d\theta \int_{0}^{2\pi} d\phi |Y_{lm}(\theta, \phi)|^2 \log |Y_{lm}(\theta, \phi)|^2 \equiv E[Y_{lm}]
\]

are the radial and angular Shannon entropies, respectively.
A posteriori observation:

The numerous properties of O.P. allow us to calculate the power (variance) and derivative (Fisher information) functionals of O.P. in an analytical way for all values of the involved quantum numbers \((n, l, m)\).

This is not the case for the logarithmic (Shannon entropy) functionals of O.P.
Application: Coulomb potential

\[ V(r) = -\frac{Z}{r} \]

(Laguerre and Gegenbauer polynomials)
Probability density in position space

\[ \rho_{nlm}(\vec{r}) = |\psi_{nlm}(\vec{r})|^2 = R^2_{nl}(r) |Y_{lm}(\theta, \phi)|^2 \]

where

\[ R^2_{nl}(r) = \frac{4}{n^4} \tilde{r}^{-1} \left[ \tilde{L}_{n-l-1}^{(2l+1)}(\tilde{r}) \right]^2 \omega_{2l+1}(\tilde{r}) \]

with

\[ \tilde{r} = \frac{2Z}{n} r \]

\[ \omega_\alpha(x) = x^\alpha e^{-x} \]
Probability density in momentum space

\[ \gamma_{nlm}(\vec{p}) = |\tilde{\Psi}_{nlm}(\vec{p})|^2 = M_{nl}^2(p) |Y_{lm}(\theta, \phi)|^2 \]

where

\[ M_{nl}^2(p) = n^3 \left( \frac{(1 + y)^3}{1 - y} \right)^{\frac{1}{2}} \left[ \tilde{C}^{(l+1)}_{n-l-1}(y) \right]^2 \omega_{l+1}^*(y) \]

with

\[ y = \frac{1 - n^2 p^2}{1 + n^2 p^2} \]

\[ \omega_{\lambda}^*(x) = (1 - x^2)^{\lambda - \frac{1}{2}} \]
Spreading measures

The Heisenberg measure

\[ V [\rho_{nlm}] := \frac{1}{4}[n^2(n^2 + 2) - l^2(l + 1)^2] \]

with

- \( n = 1, 2, \ldots \)
- \( l = 0, 1, \ldots, n - 1. \)

It doesn't depend on \( m \)
The Fisher information

\[
F[\rho_{nlm}] := 4 \left\{ \int_0^{\infty} \left\{ \frac{d}{dr} \left[ L_{n-l-1}^{(2l+1)}(r) \sqrt{\omega_{2l+1}(r)} \right] \right\}^2 dr \\
+ N_{n-l-1} \left( \int_{\Omega} \left| \frac{d}{d\theta} Y_{lm} (\theta, 0) \right|^2 d\Omega \right) \right\}
\]

\[
= \frac{4}{n^3} (n - |m|)
\]

with
- \( n = 1, 2, \ldots \)
- \( l = 0, 1, \ldots, n - 1 \)
- \( m = -l, -l + 1, \ldots, l \)

It doesn’t depend on \( l \)
The Shannon entropy

\[ S[\rho_{nlm}] = E \left[ L_{n-l-1}^{(2l+1)}(r) \right] + E \left[ Y_{lm}(\theta, \phi) \right] \]

The analytical dependence of these quantities on the quantum numbers \((n, l, m)\) is not yet analytically known except for the two extreme cases: ground state \((n = 1, l = 0, m = 0)\) and Rydberg states \((n >> 1)\), which involve polynomials and harmonics with lowest and highest orders, respectively.
Shannon entropy of the spherical harmonics

Definition

\[ E [Y_{lm}] = - \int_{\Omega} |Y_{lm}(\theta, \phi)|^2 \log |Y_{lm}(\theta, \phi)|^2 d\Omega \]

with

\[ \int d\Omega \equiv \int_{0}^{2\pi} d\phi \int_{0}^{\pi} d\theta \sin \theta \]

Exact expression by means of Gegenbauer polynomials:

\[ E [Y_{lm}] = a_{m,l} + E \left[ G_{l - |m| + \frac{1}{2}} \right] \]

\[ E \left[ G_k^\lambda \right] \equiv - \int_{-1}^{+1} \left[ G_k^\lambda(x) \right]^2 \log \left[ G_k^\lambda(x) \right]^2 \omega_\lambda(x) dx \]

denotes the entropy of the Gegenbauer polynomials, where
Coulomb potential VII

\[ G_k^\lambda(x) = \left( \frac{k!(k + \lambda)\Gamma(2\lambda)}{\lambda\Gamma(k + 2\lambda)} \right)^{\frac{1}{2}} C_k^\lambda(x) \]

\[ = \gamma_k^\lambda x^k + \text{lower degree terms} \]

which are orthogonal with respect to the positive unit weight on \([-1, +1]\),

\[ \omega_\lambda(x) = \frac{\Gamma(\lambda + 1)}{\sqrt{\pi}\Gamma(\lambda + 1/2)}(1 - x^2)^{\lambda - \frac{1}{2}} \]
The Shannon entropy of orthogonal polynomials

- Exact results
- Computation
- Asymptotics
The Shannon entropy of O.P.: Exact results I

\[ E[y_n] := - \int_a^b y_n^2(x) \log [y_n^2(x)] \omega(x) \, dx \]

This quantity has **not yet** been explicitly calculated for general orthogonal polynomials in terms of its degree \( n \) and characterizing parameters!!

There are three **beautiful exceptions**:

- Orthogonal Chebyshev polynomials of first kind \( T_n(x) \)

\[
E[T_n] = - \frac{1}{\pi} \int_{-1}^{+1} T_n^2(x) \log T_n^2(x) \frac{dx}{\sqrt{1 - x^2}}
\]

\[ = \log 2 - 1; \quad \text{for} \quad n \geq 1 \]
The Shannon entropy of O.P.: Exact results II

- Orthogonal Chebyshev polynomials of second kind \( U_n(x) \)

\[
E [U_n] = -\frac{2}{\pi} \int_{-1}^{+1} U_n^2(x) \log U_n^2(x) \sqrt{1-x^2} \, dx
\]

\[
= \frac{1}{n+1} - 1; \quad \text{for} \quad n \geq 0
\]

- Orthogonal Gegenbauer polynomials \( G_n^{(\lambda)}(x) \) for \( \lambda = 2 \)

\[
E \left[ G_n^{(2)} \right] = -\log \left( \frac{3(n+1)}{n+3} \right) - \frac{n^3 - 5n^2 - 29n - 27}{(n+1)(n+2)(n+3)}
\]

\[
- \frac{1}{n+2} \left( \frac{n+3}{n+1} \right)^{n+2}
\]
The Shannon entropy of O.P.: Computation I

How to compute (accurate and fast)

\[ E[y_n] = -\int_{\triangle} y_n^2(x) \ln y_n^2(x) \omega(x) dx \]

where \( \omega \) is a unit weight on \( \triangle = [-1, 1] \) and given \( y_n(x) = \gamma_n x^n + \ldots, \gamma_n > 0 \), satisfying

\[ \int_{\triangle} y_n(x)y_m(x)\omega(x)dx = \delta_{mn}, \quad m, n \in \mathbb{Z}_+ \]

Quadrature? Not good enough
Method based on the recurrence relations of the polynomials $y_n(x)$

First step: Define the measures

$$d\nu_n(x) = y_n^2(x) d\mu(x), \quad \lambda_n = \frac{1}{n} \sum_{j=1}^{n} \delta_{\zeta_j^{(n)}},$$

and the mutual energy of the measures $\mu$ and $\nu$

$$I[\nu, \mu] = -\int \int \ln |z - t| d\nu(t) d\mu(t),$$

and denote

$$y_n(x) = \gamma_n \prod_{j=1}^{n} \left(x - \zeta_j^{(n)}\right), \quad \gamma_n > 0.$$ 

Then,

$$E_n = -2 \ln \gamma_n + 2n I[\lambda_n, \nu_n]$$
Second step: Let us consider the Chebyshev moments of the measures $\lambda_n$ and $\nu_n$ for $k, n > 0$

$$c_{k,n} = \int T_k d\lambda_n, \quad m_{k,n} = \int T_k d\nu_n$$

Then,

$$I[\lambda_n, \nu_n] = \ln 2 + 2 \sum_{k=1}^{\infty} \frac{c_{k,n} m_{k,n}}{k}$$

where the series is convergent.

Third step: The leading coefficient $\gamma_n$ and the Chebyshev moments are evaluated from the coefficients of the three-term recurrence relation of the polynomials

$$xy_n(x) = a_{n+1}y_{n+1}(x) + b_ny_n(x) + a_ny_{n-1}(x).$$
The Shannon entropy of O.P.: Computation IV

HOW?

With $y_{-1} = 0$, $y_0(x) = 1$,

$$xy_n(x) = a_{n+1}y_{n+1}(x) + b_n y_n(x) + a_n y_{n-1}(x),$$

construct the infinite Jacobi matrix

$$J = \begin{pmatrix}
    b_0 & a_1 & 0 & 0 & \ldots \\
    a_1 & b_1 & a_2 & 0 & \ldots \\
    0 & a_2 & b_2 & a_3 & \ldots \\
    \vdots & \vdots & \vdots & \vdots & \ddots
\end{pmatrix}$$

and denote by $J_n = J(1:n, 1:n)$ its principal minor $n \times n$. 

Then

1. zeros $\zeta_{j}^{(n)}$ of $y_{n}(x)$ are eigenvalues of $J_{n}$, hence

$$\sum_{j=1}^{n} \left[ \zeta_{j}^{(n)} \right]^{m} = \text{trace of } J_{n}^{m}$$

2. following formula holds: if $f \in C(\triangle)$,

$$\int_{\triangle} f(x)y_{n}^{2}(x)\omega(x)dx = \langle f(J)e_{n+1}, e_{n+1} \rangle,$$

where $e_{n}$ is the canonical base of $l^{2}$ and $\langle \cdot, \cdot \rangle$ is the standard inner product in $l^{2}$.

3. leading coefficient $\gamma_{n} = (a_{1}a_{2}\ldots a_{n})^{-1}$. 
Algorithm

Starting from the Jacobi matrix $J$

1. find $\ln \gamma_n = - \sum_{j=1}^{n} \ln a_j$;

2. for $k \geq 1$, use the recurrence $T_{n+1}(x) = 2xT_n(x) - T_{n-1}(x)$ in order to compute
   - $c_{k,n} = \text{tr} \ T_k(J_n)$;
   - $m_{k,n} = \langle T_k(J_r) \ e_{n+1}, e_{n+1} \rangle$, \quad $r \geq n + 1 + [k/2]$,

3. gather this in

$$E[y_n] = -2 \ln \gamma_n + 2n \ln 2 + 4 \sum_{k=1}^{\infty} \frac{m_{k,n} c_{k,n}}{k}$$

truncating the series.

Advantages:

- We use only the recurrence coefficients + matrix product, nothing else.
- For lower values of $k$ (main contribution) all matrices are sparse.
The Shannon entropy of O.P.: Asymptotics I

- Jacobi polynomials $P_n^{(\alpha,\beta)}(x)$: $\omega_{\alpha,\beta}(x) = (1 - x)^{\alpha}(1 + x)^{\beta}$, $-1 \leq x \leq +1$

\[
E_n(\alpha, \beta) = \log \pi - 1 - (\alpha + \beta) \log 2 + o(1)
\]

- Laguerre polynomials $L_n^{(\alpha)}(x)$: $\omega_{\alpha}(x) = x^{\alpha}e^{-x}$, $0 \leq x < +\infty$

\[
E_n(\alpha) = -2n + (\alpha + 1) \log n - \alpha - 2 + \log \pi + o(1)
\]
Freud polynomials $F_n^{(\kappa)}(x)$: $\omega_\kappa(x) = e^{-|x|^\kappa}, \kappa < 1, \infty < x < +\infty$

\[
E_n(\kappa) = - \frac{2n + 1}{\kappa} + \frac{1}{\kappa} \log(2n) \\
- \frac{1}{\kappa} \log \left( \frac{\sqrt{\pi} \Gamma(\kappa/2)}{2 \Gamma(\kappa + 1)} \right) + \log \pi - 1 + o(1)
\]

e.g. for $\kappa = 2$ (Hermite polynomials $H_n(x)$: $\omega(x) = e^{-x^2}$)

\[
E_n(2) = -n + \log \sqrt{2n} - \frac{2}{3} + \log \pi + o(1)
\]
The Shannon entropy of O.P.: Asymptotics III

Proof

- We cannot simply substitute the asymptotics of $y_n(x)$ into the entropy functional
- The logarithmic singularity creates additional complications

We have used a methodology based on the identity

$$S[\rho] = \lim_{p \to 1} R_p[\rho]$$

for any probability density $\rho(x)$, where

$$R_p[\rho] = \frac{1}{1 - p} \log \int |\rho(x)|^p dx \quad \text{Renyi}$$

$$S[\rho] = -\int \rho(x) \log \rho(x) dx \quad \text{Shannon}$$
In our case $\rho(x) = y_n^2(x)\omega(x)$. Then,

$$E[y_n] = -\lim_{p \to 1} \frac{1}{p - 1} \log \int |y_n(x)|^{2p} \omega(x) dx$$

$$= -\lim_{p \to 1} \frac{\partial}{\partial p} N_n(2p),$$

where

$$N_n(p) := \int |y_n(x)|^p \omega(x) dx$$

denotes the $L^p(\omega)$ norms of $y_n(x)$.

**Attention:** The problem reduces to the estimation of these norms!!.
Then, the asymptotical value for the entropy is

\[ E_\infty = \lim_{n \to \infty} E[y_n] = -\lim_{n \to \infty} \frac{\partial N_n(2p)}{\partial p} \bigg|_{p=1} \]
\[ = -N'(2p) \bigg|_{p=1} \]

\[ \Rightarrow \text{ For general O.P. with weight } \omega(x) \text{ on } -1 \leq x \leq +1, \text{ one has } \]
\[ N(p) = \frac{2^{p/2} \Gamma \left( \frac{1}{2} \right) \Gamma \left( \frac{p+1}{2} \right)}{\pi^2 \Gamma \left( \frac{p+1}{2} + 1 \right)} \int_0^\pi \omega_0^{1-\frac{p}{2}}(\cos \theta) d\theta \]

with the trigonometric weight \( \omega_0 \) given by

\[ \omega_0(x) = \frac{\omega(x)}{\omega_C(x)}; \quad \omega_C(x) \equiv \frac{1}{\pi} \frac{1}{\sqrt{1-x^2}} \]

End of proof
Matrix mechanics
and
new discrete entropies of orthogonal polynomials
as well as
the entropy of a matrix
A mechanical observable of a system in the matrix formulation of Q.M. is expressed by

$$
\hat{O}_n = \begin{pmatrix}
  a_1 & b_1 \\
  b_1 & a_2 & b_2 \\
  & \ddots & \ddots & \ddots \\
  & & \ddots & \ddots & b_{n-1} \\
  & & & b_{n-1} & a_n
\end{pmatrix}
$$

Quantum predictions:

$$
\det(\hat{O}_n - \lambda I) = 0 \Rightarrow \lambda = \lambda_k^{(n)}; k = 1, 2, \ldots, n
$$
Discrete entropies of orthogonal polynomials II

The eigenvectors
\[ \vec{p}(\lambda_k^{(n)}) = \left[ p_0, p_1(\lambda_k^{(n)}), \ldots, p_{n-1}(\lambda_k^{(n)}) \right]^T \equiv \left[ p_{i-1}(\lambda_k^{(n)}) \right]_{i=1}^n \]
are the solutions of
\[ \hat{O}_n \vec{p}(\lambda_k^{(n)}) = \lambda_k^{(n)} \vec{p}(\lambda_k^{(n)}) \]
where \( \{p_i(\lambda)\}_{i=0}^{n-1} \) forms an orthonormal polynomial system with TTRR
\[ \lambda p_i(\lambda) = b_{i+1} p_{i+1}(\lambda) + a_{i+1} p_i(\lambda) + b_i p_{i-1}(\lambda); \ i = 0, 1, \ldots, n - 2 \]

Normalized eigenvectors:
\[ \vec{\psi}(\lambda_k^{(n)}) = \sqrt{l_n(\lambda_k^{(n)})} \vec{p}(\lambda_k^{(n)}) \equiv \left[ \psi_i(\lambda_k^{(n)}) \right]_{i=1}^n \]
with the Christoffel function
\[ l_n(\lambda) := \frac{1}{\langle \vec{p}_i, \vec{p}_i \rangle} = \frac{1}{\sum_{i=0}^{n-1} p_i^2(\lambda)} \]
Discrete entropies of orthogonal polynomials III

Let us now consider the $n \times n$ orthogonal matrix

$$
\Psi = [\psi_{ij}]_{i,j=1}^n \equiv \left[ \psi_i \left( \lambda_j^{(n)} \right) \right]_{i,j=1}^n = \left[ \sqrt{l_n(\lambda_j^{(n)})} p_{i-1}^{(n)}(\lambda_j^{(n)}) \right]_{i,j=1}^n
$$

which is made of the $n \times 1$ column matrices

$$
\vec{\psi}(\lambda_j^{(n)}) = [\psi_i^{(n)}]_{i=1}^n \equiv [\psi_{ij}]_{i=1}^n.
$$

Then, the distribution $\{\psi_1^2, \psi_2^2, \ldots, \psi_n^2\}$ with

$$
\psi_i^2 = \psi_i^2 \left( \lambda_j^{(n)} \right) = l_n \left( \lambda_j^{(n)} \right) p_{i-1}^2 \left( \lambda_j^{(n)} \right) \quad (1)
$$

gives a discrete probability density. The Shannon entropy of this density is

$$
S_{n,j} := - \sum_{i=1}^n \psi_i^2 \left( \lambda_j^{(n)} \right) \log \psi_i^2(\lambda_j^{(n)}); \quad j = 1, \ldots, n \quad (2)
$$

Note that the summation does not run on the argument $\lambda$ of $\psi$. 

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From (1) and (2), one has

\[ S_{n,j} \equiv S_n \left( \lambda_j^{(n)} \right) = -\log l_n \left( \lambda_j^{(n)} \right) - l_n \left( \lambda_j^{(n)} \right) \sum_{i=1}^{n} p_{i-1}^2 \left( \lambda_j^{(n)} \right) \log p_{i-1}^2 \left( \lambda_j^{(n)} \right) \]

This can be generalized as follows

\[ S_n(\lambda) := -\log(l_n(\lambda)) - l_n(\lambda) \sum_{i=1}^{n} p_{i-1}^2 (\lambda) \log p_{i-1}^2 (\lambda) \]

which is the new discrete entropy of orthogonal polynomials.
Applications:

(i) Orthonormal Chebyshev polynomials of first kind.

\[ S_{n,j} \equiv S_n \left( \lambda_j^{(n)} \right) = \log n + \log 2 - 1 + \frac{\log 2}{n} + R \left( \frac{d}{2n} \right) \]

where \( d = \text{GCD}(2j - 1, n) \), and

\[ R(x) = x[\psi(1 - x) + 2\gamma + \psi(1 + x)]; x \in [0, 1) \]

\[ = -2 \sum_{k=1}^{\infty} \zeta(2k + 1)x^{2k+1} \]

where \( \gamma \) is the Euler’s constant, \( \psi(x) = \Gamma'(x)/\Gamma(x) \) the digamma function, and \( \zeta(\cdot) \) is the Riemann zeta function. The Taylor series expansion is absolutely convergent for \(|x| < 1\).
(ii) Orthonormal Chebyshev polynomials of second kind

\[ S_{n,j} = \log(n + 1) + \log 2 - 1 + R \left( \frac{d}{n + 1} \right); \quad d = \text{GCD}(j, n + 1) \]

⇒ The leading term \( \log n \) in both cases shows that the values

\[ p_0^2, p_1^2(\lambda_k^{(n)}), \ldots, p_{n-1}(\lambda_k^{(n)}), \]

normalized by an appropriate factor, are approximately equidistributed.
The dual discrete entropy of orthogonal polynomials

- **The dual discrete entropy:**
  Since $\Psi$ is an orthogonal matrix, its rows

  \[
  \left[ \psi_{i-1} \left( \lambda_k^{(n)} \right) \right]_{k=1}^n \equiv \left[ \sqrt{l_n(\lambda_1^{(n)})} p_{i-1} \left( \lambda_1^{(n)} \right), \ldots, \sqrt{l_n(\lambda_n^{(n)})} p_{i-1} \left( \lambda_n^{(n)} \right) \right]
  \]

  are also orthogonal vectors of $\mathbb{R}^n$:

  \[
  \delta_{ij} = \sum_{k=1}^n l_n \left( \lambda_k^{(n)} \right) p_{i-1} \left( \lambda_k^{(n)} \right) p_{j-1} \left( \lambda_k^{(n)} \right) = \int p_{i-1}(\lambda) p_{j-1}(\lambda) d\mu_n(\lambda)
  \]

  where $\mu_n$ is the normalized counting measure of zeros of $p_n$:

  \[
  \mu_n = \sum_{k=1}^n l_n \left( \lambda_k^{(n)} \right) \delta_{\lambda_k^{(n)}}
  \]
Hence, we may define the dual discrete entropy as

\[ S_n^i = - \sum_{j=1}^{n} \psi_{i-1}^2 \left( \lambda_j^{(n)} \right) \log \psi_{i-1}^2 \left( \lambda_j^{(n)} \right) \]

\[ = - \sum_{j=1}^{n} \left[ \ln \left( \lambda_j^{(n)} \right) p_{i-1}^2 \left( \lambda_j^{(n)} \right) \right] \log \left[ \ln \left( \lambda_j^{(n)} \right) p_{i-1}^2 \left( \lambda_j^{(n)} \right) \right] \]

for \( i = 1, \ldots, n \).
The entropy of an orthogonal matrix $\Psi$ is defined as

$$S(\Psi) = -\sum_{i=1}^{n} \sum_{j=1}^{n} \psi_{ij}^2 \log \psi_{ij}^2$$

Here, $\psi_{ij}$'s are real numbers with the orthogonality constraint

$$\sum_{i=1}^{n} \psi_{ij} \psi_{ik} = \delta_{jk}$$

General remark:

$$0 \leq S(\Psi) \leq n \log n$$

The minimum value zero is attained by the identity matrix, i.e. for

$$\Psi = I = [\delta_{ij}]_{i,j=1}^{n}$$
The entropy of an orthogonal matrix II

The entropy of the $i$th-row can have the maximum value $\log n$, which is attained when each element of the row is $\pm \frac{1}{\sqrt{n}}$. This gives the upper bound $n \log n$, which is obtained only by the Hadamard matrices (rescaled by $n^{-\frac{1}{2}}$).

The Hadamard matrices $H_n$ are orthogonal matrices up to a proportional factor $\sqrt{n}$:

$$H_n H_n^T = nI_n$$

and have elements $\pm 1$.

So, the Hadamard matrices can be interpreted as the orthogonal matrices which saturate the bound $n \log n$ for this entropy.
Conclusions
Conclusions I

1. The information-theoretic entropies (Fisher, Shannon) of quantum systems boil down to the corresponding entropies of some special functions (often, orthogonal polynomials)
   - The Fisher information of classical O.P. can be explicitly evaluated.
   - The Shannon entropy of classical O.P. cannot be analytically calculated. A recurrence-based algorithm for its computation has been designed. Moreover, its asymptotics has been obtained in full detail.

2. A discrete entropy (and its dual) of O.P. has been proposed, and illustrated in the Chebyshev case.

3. It has been introduced the notion of matricial entropy, whose properties need to be explored.
Conclusions II

- Cramer-Rao information plane of the Jacobi orthogonal polynomials

For $n = 0, 1, 2, 3$.

Variation of $\alpha$ and $\beta$. 

![Graph showing variations of $\alpha$ and $\beta$.](image)
Conclusions III

- Cramer-Rao information plane of the classical orthogonal polynomials (Jacobi, Laguerre, Hermite)
Information-theoretic comparative study of the classical orthogonal polynomials

\[ \rho_n(x) = p_n^2(x) \omega(x) \]

<table>
<thead>
<tr>
<th>Polynomial</th>
<th>Variance $V$</th>
<th>Fisher information $I$</th>
<th>Shannon entropy power $N$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Hermite $H_n(x)$</td>
<td>$\sim n$</td>
<td>$\sim 4n$</td>
<td>$\sim n$</td>
</tr>
<tr>
<td>Laguerre $L_n^{\alpha}(x)$</td>
<td>$\sim 2n$</td>
<td>( \begin{cases} \sim \frac{2n}{\alpha} \ \sim \infty (\alpha \to 1) \ \sim 0 (\alpha \to \infty) \end{cases} )</td>
<td>( \begin{cases} \sim n^2 (\alpha \text{ fixed}) \ \sim \alpha (n \text{ fixed}) \end{cases} )</td>
</tr>
<tr>
<td>Jacobi $P_n^{\alpha,\beta}(x)$</td>
<td>$\sim 1/2$</td>
<td>$\sim c(\alpha, \beta)n^3$</td>
<td>( \begin{cases} \swarrow (\alpha, \beta \text{ fixed}) \ \nearrow (n, \beta \text{ fixed}) \end{cases} )</td>
</tr>
</tbody>
</table>