Medidas de complejidad de polinomios ortogonales

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Motivation

Michel Baranger (M.I.T., N.E.C.S.I., USA) *dixit*:

Twentieth-century theoretical physics came out of the relativistic revolution and the quantum mechanical revolution. It was all about simplicity and continuity (in spite of quantum jumps).

- Its principal tool was calculus.
- Its final expression was field theory.

Twenty-first-century theoretical physics is coming out of the chaos revolution.

- It will be about complexity and its principal tool will be the computer.
- Its final expression remains to be found.

Motivation

Murray Gell-Mann (1969 Nobel Prize for Physics) *dixit*:

Our world can be seen as a huge complex system consisting of an enormous number of interacting natural, social and artificial complex systems.

We cannot successfully analyse this system by determining in advance a set of properties or aspects that are studied separately and then recombining those partial approaches in an attempt to form a picture of the whole.

Instead, it is necessary to look at the whole system, even if it means taking a crude look, and then allowing possible simplifications to emerge from the work.

Quantifying complexity

Contemporary researchers in architecture, biology, computer science, dynamical systems, engineering, finance, game theory, etc., have defined different measures of complexity for each field.

Three questions that researchers frequently ask to quantify the complexity of the thing (house, bacterium, computer problem, technological process, investment scheme, ...) under study are

- How hard is it to describe?
- How hard is it to create?
- What is its degree of organization?

Classifying complexity

To a large extent all the measures of complexity can be grouped in two groups:

- *Extrinsic measures*: they do depend on the context, such as e.g. the algorithmic and computational complexities; they are closely related to the time required for a computer to solve a given problem; so that it depends on the chosen computer.
- *Intrinsic measures*: they do not depend on the context but on the probability density of the system under consideration

General purpose

To quantify how simple or how complex are the special functions of Applied Mathematics, beginning by the classical or hypergeometric-type orthogonal polynomials in a real continuous variable.

The issues

- How do we understand by simplicity and complexity?
- In what sense a certain mathematical function is simple and complex another one?

are not at all simple.

There does not exist a unique notion of complexity to grasp our intuitive notions in the appropriate manner.

Specific aim

To quantify how simple or how complex are the classical orthogonal polynomials $p_n(x)$ *by means of the complexity measures of its associated Rakhmanov probability density.*

Remark that, contrary to other complexity notions (algorithmic, computational,...), the density-dependent complexities are intrinsic properties of the polynomials.

Thus, the intrinsic complexity notions are closely related to the main *macroscopic features* of the associated probability density of the polynomials (irregularities, extent, fluctuations, smoothing,...).

Entropy measures

Ordinary moments

$$\langle r^k \rangle = \int r^k \rho(\mathbf{x}) d\mathbf{x}; \;\; k = 0, 1, 2, \ldots; \;\; r \equiv |\mathbf{x}|$$

$$\Longrightarrow \text{Variance } V[\rho] = \langle r^2 \rangle - \langle r \rangle^2$$

Entropy moments

$$W_q[\rho] = \int [\rho(\mathbf{x})]^q \, d\mathbf{x} = \langle \rho^{q-1} \rangle; \;\; q \geq 1$$

$$\Longrightarrow \text{Rényi entropy } R_q[\rho] = \frac{1}{1-q} \ln \int [\rho(\mathbf{x})]^q \, d\mathbf{x}$$

Shannon entropy

$$S[\rho] = \int \rho(\mathbf{x}) \log \rho(\mathbf{x}) d\mathbf{x}$$

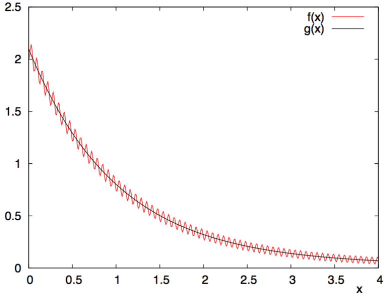
Fisher information

$$F[\rho] = \int \frac{|\nabla \rho(\mathbf{x})|^2}{\rho(\mathbf{x})} d\mathbf{x}$$

Comparación entrópica en densidades sencillas:

e.g.,

$$g(x) \sim e^{-ax}, \qquad f(x) \sim e^{-ax} + \epsilon \sin^2(nx)$$



Función	Entropía Shannon	Varianza	Desequilibrio	Información Fisher
$g(x)$	1.3485	0.07962	0.2690	9.3×10^{-1}
$f(x)$	1.3476	0.07966	0.2695	3.7×10^{3}

Complexity measures

Fisher-Shannon complexity

$$C_{\mathsf{FS}}[\rho] = F[\rho] \times \frac{1}{2\pi e} \exp\left(2\, S[\rho]\right)$$

LMC complexity

$$C_{\mathsf{LMC}}[\rho] = W_2[\rho] \times \exp\left(S[\rho]\right)$$

Crámer-Rao complexity

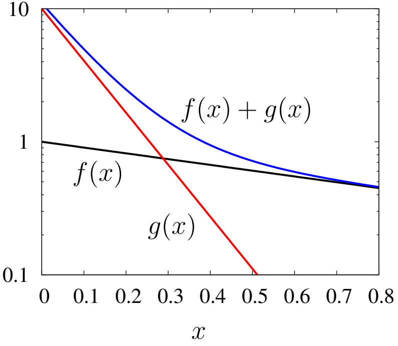
$$C_{\mathsf{CR}}[\rho] = F[\rho] \times V[\rho]$$

Some properties:

- Invariance under replication, translation and scaling transformations.
- Minimal values at the two extreme cases:
    - completely ordered systems (e.g. Dirac delta distribution)
    - totally disordered systems (e.g. uniform distribution)

Remark:

The complexity measures quantify how easily a system may be modelled!

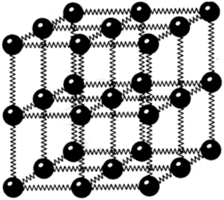


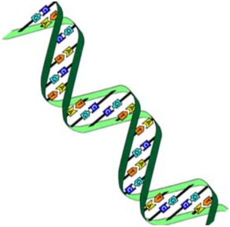
$$f(x) \sim e^{-ax}$$

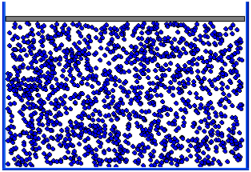
$$g(x) \sim e^{-bx}$$

What does complexity really mean in 3D?

Complexity measures how easily modelling a system may be.







From a physical point of view, a *completely ordered system* (e.g., a perfect cristal with high internal structure) as well as a *totally disordered one* (e.g., an isolated ideal gas), are not complex systems.

Between these two extreme cases, we find many others in which order and disorder are involved simultaneously.

Rakhmanov density of orthogonal polynomials

The spread of the hypergeometric orthogonal polynomials $\{p_n(x)\}$ satisfying

$$\int_\Omega p_n(x)\, p_m(x)\, \omega(x)\, dx = d_n^2\, \delta_{mn}$$

is given by the distribution of its associated Rakhmanov probability density

$$\rho_n(x) = \frac{1}{d_n^2}\, p_n^2(x)\, \omega(x)$$

Entropic moments of P.O.s

The qth-power of the weighted L_q-norm is called *entropic moment* W_q:

$$W_q[\rho_n^{(\{\alpha\})}] = \int_\Delta \left(\rho_n^{(\{\alpha\})}(x)\right)^q dx = \int_\Delta \left(\left(p_n^{(\{\alpha\})}(x)\right)^2 \omega_{\{\alpha\}}(x)\right)^q dx,$$

which are closely related to the *Rényi entropy*:

$$R_q[\rho_n^{(\{\alpha\})}] = \frac{1}{1-q} \ln W_q[\rho_n^{(\{\alpha\})}]; \quad q > 0, q \neq 1,$$

The well-known *Shannon entropy* is the limiting case

$$\lim_{q \to 1} R_q[\rho_n^{(\{\alpha\})}] = S[\rho_n^{(\{\alpha\})}] = \int_\Delta \rho_n^{(\{\alpha\})}(x) \ln \rho_n^{(\{\alpha\})}(x) dx.$$

Methodology:

To evaluate the L_q-norms (or its qth-powers, the entropic moments) of the real continuous orthogonal polynomials we use the linearization technique:

$$\left(\left(p_n^{(\{\alpha\})}(x)\right)^2\right)^q = \sum_{i=0}^{\infty} c_i \; p_i^{(\{\beta\})}(x),$$

whose coefficients c_i can be expressed in terms of multivariate

hypergeometric functions.

Linearization of the power of a polynomial

Our problem is to find the coefficients c_i of the series such as

$$\left(\left(p_n^{(\{\alpha\})}(x)\right)^2\right)^q = \sum_{i=0}^{\infty} c_i \; p_i^{(\{\beta\})}(x),$$

for any real $q > 0$.

However, with the techniques we have up to now, we can obtain these expansions *only for positive integer powers* $2q \in \mathbb{N}$:

$$\left(p_n^{(\{\alpha\})}(x)\right)^{2q} = \sum_{i=0}^{\infty} c_i \; p_i^{(\{\beta\})}(x).$$

Linearization of Laguerre polynomials

We use the H.M. Srivastava linearization [1988]:

$$x^{\mu}\left(L_n^{(\alpha)}(tx)\right)^r=\sum_{i=0}^{\infty}c_i(\mu,r,t,n,\alpha,\gamma)\;L_i^{(\gamma)}(x),$$

where the coefficients $c_i(\mu,r,t,n,\alpha,\gamma)$ are expressed as:

$$c_i(\mu,r,t,n,\alpha,\gamma)=(\gamma+1)_\mu\binom{n+\alpha}{n}^r \times F_A^{(r+1)}\left(\begin{array}{c}\gamma+\mu+1;\overbrace{-n,\ldots,-n}^{r},-i\\ \underbrace{\alpha+1,\ldots,\alpha+1}_{r},\gamma+1\end{array};\overbrace{t,\ldots,t}^{r},1\right),$$

where $F_A^{(r+1)}$ is a Lauricella function of type A of $r+1$ variables.

Definition: The *Lauricella function of type* A of s variables is

$$F_A^{(s)}\left(\begin{array}{c} a; b_1, \ldots, b_s \\ c_1, \ldots, c_s \end{array}; x_1, \ldots, x_s\right) = \sum_{j_1, \ldots, j_s = 0}^{\infty} \frac{(a)_{j_1+\cdots+j_s} (b_1)_{j_1} \cdots (b_s)_{j_s}}{(c_1)_{j_1} \cdots (c_s)_{j_s}} \frac{x_1^{j_1} \cdots x_s^{j_s}}{j_1! \cdots j_s!}.$$

It is a generalization of the *Appell function* F_2 of two variables.

Entropic moments of Laguerre polynomials

Now, we apply the linearization

$$y^{\alpha q}\left(L_n^{(\alpha)}\left(\frac{y}{q}\right)\right)^{2q}=\sum_{i=0}^{\infty}\Gamma(\alpha q+1)\binom{n+\alpha}{\alpha}^{2q}$$

$$\times F_A^{(2q+1)}\left(\begin{array}{c}\alpha q+1;-n,\ldots,-n,-i\\ \alpha+1,\ldots,\alpha+1,1\end{array};\frac{1}{q},\ldots,\frac{1}{q},1\right)L_i^{(0)}(y).$$

Entropic moment of order q of Laguerre polynomials

$$W_q[\rho_n^{(\alpha)}]=\frac{\Gamma(\alpha q+1)}{q^{\alpha q+1}}\left(\frac{\Gamma(n+\alpha+1)}{n!\,(\Gamma(\alpha+1))^2}\right)^q$$

$$\times F_A^{(2q)}\left(\begin{array}{c}\alpha q+1;-n,\ldots,-n\\ \alpha+1,\ldots,\alpha+1\end{array};\frac{1}{q},\ldots,\frac{1}{q}\right)$$

Crámer-Rao complexity of Laguerre polys

The Rakhmanov probability density of the Laguerre polynomials $L_n^{(\alpha)}(x)$ characterized by the orthogonality condition

$$\int_0^{+\infty} L_n^{(\alpha)}(x) L_m^{(\alpha)}(x) x^\alpha e^{-x} dx = \delta_{mn},$$

is defined by

$$\rho_L(x) = \left[L_n^{(\alpha)}(x)\right]^2 x^\alpha e^{-x}.$$

Then, the Crámer-Rao complexity of the Laguerre polynomials is given by

$$C_{CR}[\rho_L] = F[\rho_L] \times V[\rho_L], \tag{1}$$

where the variance is given by

$$V[\rho_L] = 2n^2 + 2(\alpha+1)n + \alpha + 1, \tag{2}$$

and the Fisher information has the value

$$F[\rho_L] = \begin{cases} 4n+1, & \alpha = 0, \\ \frac{(2n+1)\alpha+1}{\alpha^2-1}, & \alpha > 1, \\ \infty, & \alpha \in [-1,+1], \alpha \neq 0, \end{cases} \tag{3}$$

respectively. Then one obtains the following value

$$C_{CR}[\rho_L] = \begin{cases} 8n^3 + [8(\alpha+1)+2]\,n^2 + 6(\alpha+1)n + (\alpha+1), & \alpha = 0, \\ \frac{1}{\alpha^2-1}\left[4\alpha n^3 + (4\alpha^2+6\alpha+2)n^2 + (4\alpha^2+6\alpha+2)n + (\alpha+1)^2\right], & \alpha > 1, \\ \infty, & \text{otherwise}, \end{cases}$$

for the Crámer-Rao complexity of Laguerre polynomials.

Fisher-Shannon complexity of Laguerre polys

Definition:

$$C_{FS}[\rho_L] = F[\rho_L] \times \frac{1}{2\pi e} \exp(2\, S[\rho_L]), \tag{4}$$

where the Shannon length or Shannon entropy power $N[\rho_L] = \exp(S[\rho_L])$ is not yet known for all values of the degree n.

However, its asymptotics (large n) has been found to be

$$N[\rho_L] \approx \frac{2\pi n}{e}. \tag{5}$$

Then, Eqs.(3), (4) and (5) gives the following asymptotics for the Fisher-Shannon complexity of the Laguerre polynomial $L_n^{(\alpha)}(x)$:

$$C_{FS}[\rho_L] \approx \begin{cases} \left(\frac{8\pi}{e^3}\right) n^3, & \alpha = 0, \\ \frac{4\alpha}{\alpha^2-1} \left(\frac{\pi}{e^3}\right) n^3, & \alpha > 1, \\ \infty, & \text{otherwise.} \end{cases}$$

LMC complexity of Laguerre polys

Definition:

$$C_{LMC}[\rho_L] = W_2[\rho_L] \times \exp(S[\rho_L]).$$

where

- the Shannon length $N[\rho_L]$ is only known in the asymptotic case (see Eq.5), while
- the second-order entropic moment $W_2[\rho_L]$ has been recently shown to be expressed in two following ways for all values of the degree n:
  - (i) In terms of the four-variate Lauricella function $F_A^{(4)}\left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right)$
  - (ii) In terms of the multivariate Bell polynomials $B_{m,l}(a_1, a_2 \ldots, a_{m-l+1})$

Indeed,

(i) In terms of the four-variate Lauricella function $F_A^{(4)}\left(\frac{1}{2},\frac{1}{2},\frac{1}{2},\frac{1}{2}\right)$:

$$W_2[\rho_L] = \left(\frac{n!}{\Gamma(\alpha+n+1)}\right)^2 \frac{\Gamma(2\alpha+1)}{2^{2\alpha+1}} \binom{n+\alpha}{n}^4 \times F_A^{(4)}\left(\begin{array}{c} 2\alpha+1; -n,-n,-n,-n \\ \alpha+1,\alpha+1,\alpha+1,\alpha+1 \end{array}; \frac{1}{2},\frac{1}{2},\frac{1}{2},\frac{1}{2}\right). \quad (6)$$

(ii) In terms of the multivariate Bell polynomials $B_{m,l}(a_1, a_2 \ldots, a_{m-l+1})$:

$$W_2[\rho_L] = \left[\sum_{k=0}^{4n} \frac{\Gamma(2\alpha+k+1)}{2^{2\alpha+k+1}} \frac{(4)!}{(k+4)!} B_{k+4,4}\left(c_0^{(n,\alpha)}, 2!c_1^{(n,\alpha)}, ..., (k+1)!c_k^{(n,\alpha} \right.\right. \quad (7)$$

where the parameters $c_t^{(n,\alpha)}$ are given by

$$c_t^{(n,\alpha)} = \sqrt{\frac{\Gamma(n+\alpha+1)}{n!}} \frac{(-1)^t}{\Gamma(\alpha+t+1)} \binom{n}{t}.$$

Numerics-1: Crámer-Rao complexity of HOPs. w.r.t. n

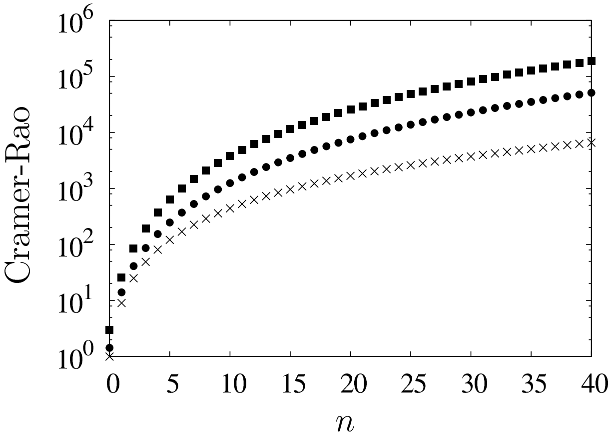


Figure : Crámer-Rao complexity measure for the Rakhmanov densities of the Hermite $H_n(x)$ ($\times$), Laguerre $L_n^{(2)}(x)$ (■) and Jacobi $P_n^{(2,2)}(x)$ (•) polynomials as a function of the degree n for $n = 0, 1, \ldots, 40$.

Numerics-2: Fisher-Shannon complexity of HPOs. w.r.t. n

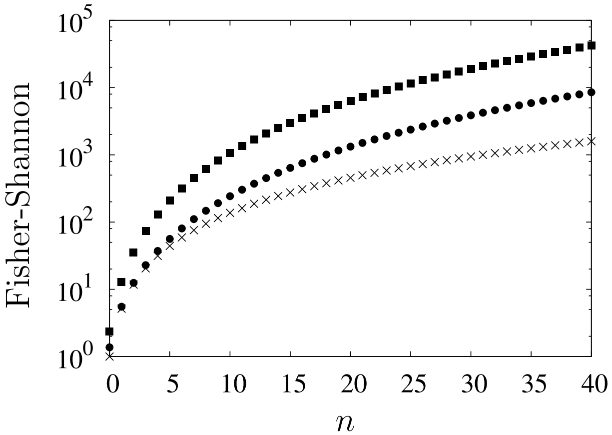


Figure : Fisher-Shannon complexity measure for the Rakhmanov densities of the Hermite $H_n(x)$ (×), Laguerre $L_n^{(2)}(x)$ (■) and Jacobi $P_n^{(2,2)}(x)$ (•) polynomials as a function of the degree n for $n = 0, 1, \ldots, 40$.

Numerics-3: LMC complexity of HPOs. w.r.t. n

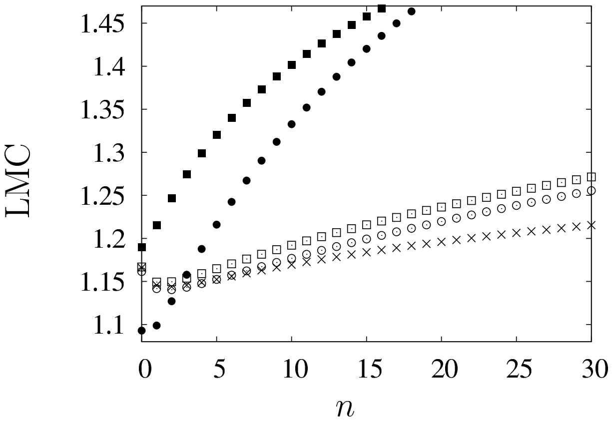


Figure : LMC complexity measure for the Rakhmanov densities of the Hermite $H_n(x)$ ($\times$), Laguerre $L_n^{(2)}(x)$ (■) and $L_n^{(50)}(x)$ (□), and Jacobi $P_n^{(2,2)}(x)$ ($\bullet$) and $P_n^{(50,50)}(x)$ ($\circ$) polynomials, as a function of the degree n for $n = 0, 1, \ldots, 30$.

Numerics-4: Crámer-Rao complexity HPOs. w.r.t. α

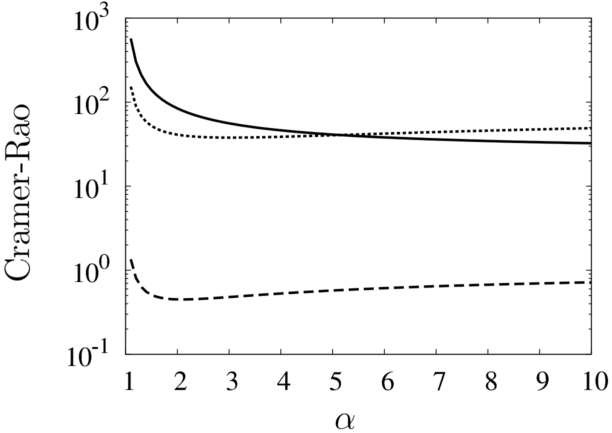


Figure : Crámer-Rao complexity measure for the Rakhmanov densities of the Laguerre $L_2^{(\alpha)}(x)$ (solid line), and the Jacobi $P_0^{(\alpha,0)}(x)$ (dashed line) and $P_2^{(\alpha,2)}(x)$ (dotted line) polynomials, as a function of the parameter α, for $1 \leq \alpha \leq 10$

Numerics-5: Fisher-Shannon complexity of HPOs. w.r.t. α

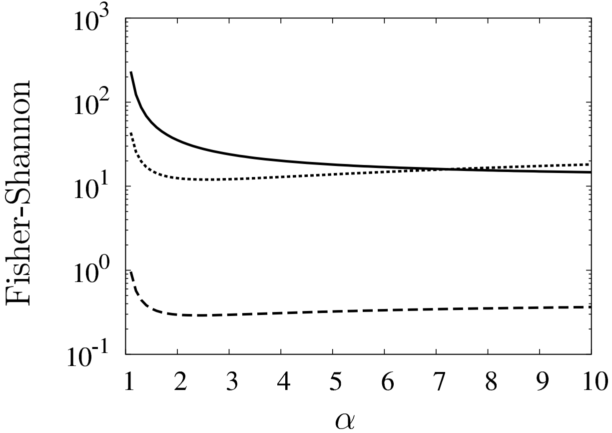


Figure : Fisher-Shannon complexity measure for the Rakhmanov densities of the Laguerre $L_2^{(\alpha)}(x)$ (solid line), and the Jacobi $P_0^{(\alpha,0)}(x)$ (dashed line) and $P_2^{(\alpha,2)}(x)$ (dotted line) polynomials, as a function of the parameter α, for $1 \leq \alpha \leq 10$

Numerics-6: LMC complexity of HPOs. w.r.t. α

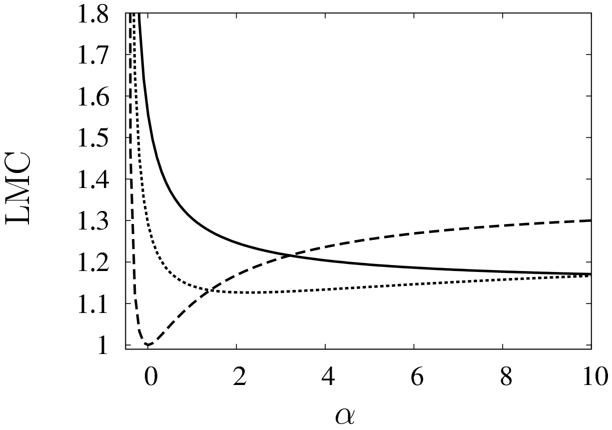


Figure : LMC complexity measure for the Rakhmanov densities of the Laguerre $L_2^{(\alpha)}(x)$ (solid line), and the Jacobi $P_0^{(\alpha,0)}(x)$ (dashed line) and $P_2^{(\alpha,2)}(x)$ (dotted line) polynomials, as a function of the parameter α, for $-\frac{1}{2} < \alpha < 10$.

Hydrogenic Schrödinger equation

$$\left[\frac{1}{2}\vec{\nabla}^2 + V(\vec{r})\right]\Psi_{nlm}(\vec{r}) = E_n\Psi_{nlm}(\vec{r}) \tag{8}$$

Quantum states for the Coulomb potential $V(\vec{r}) = -\frac{Z}{r}$

- Energies: $E_n = -\frac{Z^2}{2n^2}$
- Probability density: $\rho_{nlm}(\vec{r}) = |\Psi_{nlm}(\vec{r})|^2 = R^2_{nl}(r)\ |Y_{lm}(\theta,\phi)|^2$
  where

$$R^2_{nl}(r) = \frac{4Z^3}{n^4}\tilde{r}^{-1}\omega_{2l+1}(\tilde{r})\left[\tilde{L}^{(2l+1)}_{n-l-1}(\tilde{r})\right]^2$$

  with

$$\tilde{r} = \frac{2Z}{n}r; \qquad \omega_\alpha(x) = x^\alpha e^{-x}$$

Hydrogenic spreading measures

- The Heisenberg measure

$$V\left[\rho_{nlm}\right] = \frac{1}{4Z^3}\left[n^2(n^2+2) - l^2(l+1)^2\right]$$

with

- $n = 1, 2, ...$
- $l = 0, 1, .., n-1.$

It doesn't depend on $\mathbf{m}$

Entropy measures

- The Fisher information

$$F[\rho_{nlm}] = 4\left\{\int_0^\infty \left\{\frac{d}{dr}\left[\sqrt{\omega_{2l+1}}L_{n-l-1}^{(2l+1)}\right]\right\}^2 dr + N_{n-l-1}\int_\Omega \left|\frac{d}{d\theta}Y_{lm}(\theta,0)\right|^2 d\Omega\right\} = \frac{4Z^3}{n^3}(n-|m|)$$

with

- $n = 1, 2, ...$
- $l = 0, 1, .., n-1.$
- $m = -l, -l+1, ..., l$

It doesn't depend on l

- The Shannon entropy

$$S[\rho_{nlm}] = S[R_{nl}] \times S[Y_{lm}]$$
$$= A(n,l,m) + \frac{1}{2n} E_1 \left[L_{n-l-1}^{(2l+1)} \right] + E \left[C_{n-|m|}^{(|m|+\frac{1}{2})} \right] - 3 \log Z$$

where the entropic integrals

$$E_i[p_k] := -\frac{1}{\pi} \int_a^b x^i p_k^2(x) \log \left[p_k^2(x) \right] \omega(x) dx; \quad i = 0, 1$$

cannot be explicitly calculated except in the two cases:

Circular states $(n, l = m = n-1)$

Rydberg states (large and very large n)

In particular

$$S[\rho_{100}] = 3 + \log \pi - 3 \log Z \qquad \text{for the Ground state}$$

and

$$S[\rho_{n00}] = 6 \log n - \log 2 + 2 \log \pi + o(1) \qquad \text{for (ns) Rydberg states}$$

Complexity measures

- Cramér-Rao complexity

$$C_{\mathrm{CR}}[\rho_{nlm}] := F[\rho_{nlm}] \times V[\rho_{nlm}]$$
$$= \frac{n-|m|}{n^3}\left(n^2(n^2+2) - l^2(l+1)\right)^2$$

- LMC shape complexity

$$C_{\mathrm{LMC}}[\rho_{nlm}] := \langle \rho_{nlm} \rangle \times \exp\left(S[\rho_{nlm}]\right)$$

Since $\langle \rho_{nlm} \rangle = Z^3 D(n,l,m)$ one has

$$C_{\mathrm{LMC}}[\rho_{nlm}] = D(n,l,m) e^{B(n,l,m)}$$

where

$$B(n,l,m) = A(n,l,m) + \frac{1}{2n} E_1\left[L_{n-l-1}^{(2l+1)}\right] + E\left[C_{n-|m|}^{(|m|+\frac{1}{2})}\right]$$

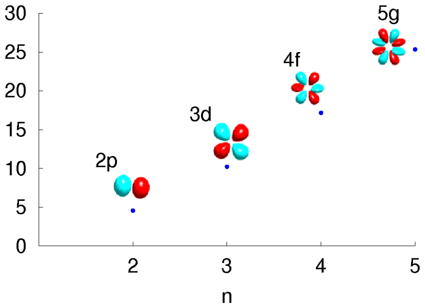
and

$A(n,l,m)$ and $D(n,l,m)$ are explicitly known

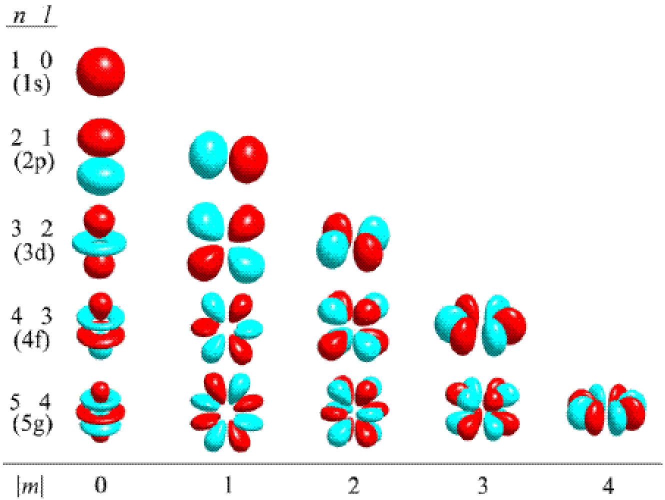
- Fisher-Shannon complexity

$$C_{\mathsf{FS}}[\rho_{nlm}] := F[\rho_{nlm}] \times \frac{1}{2\pi e} \exp\left(\frac{2}{3} S[\rho_{nlm}]\right)$$
$$= \frac{4(n-|m|)}{n^3} \frac{1}{2\pi e} e^{\frac{2}{3} B(n,l,m)}$$

For quasicircular states $(n, l = n-1)$,



Quasicircular states $(n, l = n - 1)$



Hydrogenic complexity remarks

- The three complexity measures do not depend on Z!!!
- Dependence on the quantum numbers (n, l, m)
  - All increase with increasing n for (l, m) fixed.
  - All decrease with increasing l for (n, m) fixed.
  - All decrease with increasing m for (n, l) fixed.

Entropic and complexity measures of the ground state hydrogenic atom $(n = 1, l = m = 0)$*:*

- Entropic measures

  Shannon entropy

$$S[\rho_{100}] = 3 + \log \pi - 3 \log Z$$

  Fisher information

$$F[\rho_{100}] = 4Z^2$$

- Complexity measures

  Cramér-Rao

$$C_{\mathsf{CR}}[\rho_{100}] = 3$$

  LMC shape

$$C_{\mathsf{LMC}}[\rho_{100}] = \frac{e^3}{8}$$

  Fisher-Shannon

$$C_{\mathsf{FS}}[\rho_{100}] = \frac{2e}{\pi^{1/3}}$$

Conclusions

- We have obtained the weighted L_q norms ($q \in \mathbb{N}$) and complexity measures of the Rahkmanov densities associated to the Hermite, Laguerre and Jacobi orthogonal polynomials.
- They were expressed in terms of *Lauricella functions* of type F_A for the Hermite and Laguerre polynomials, and in terms of a *Srivastava-Daoust function* for the Jacobi polynomial.
- These expressions, together with the monotonicity of the information-theoretic Rényi entropy, have been used to obtain bounds on the Lauricella and Srivastava-Daoust functions.

Open problems (Math.)

- Search for recurrence formulas of these norms.
- Reduction of the involved Lauricella and Srivastava-Daoust functions, which will conduct to simpler expressions of the L_q norms and complexity measures for the hypergeometric OPs.
- Calculation of the exact expressions of the L_q norms for $q \in \mathbb{R}$.
- Extensions of these results to special functions other than the hypergeometric OPs..