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Asymptotics of orthogonal polynomial's entropy

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Dedicated to Professor Jesús S. Dehesa on the occasion of his 60th birthday.

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ABSTRACT

This is a brief account on some results and methods of the asymptotic theory dealing with the entropy of orthogonal polynomials for large degree. This study is motivated primarily by quantum mechanics, where the wave functions and the densities of the states of solvable quantum-mechanical systems are expressed by means of orthogonal polynomials. Moreover, the uncertainty principle, lying in the ground of quantum mechanics, is best formulated by means of position and momentum entropies. In this sense, the behavior for large values of the degree is intimately connected with the information characteristics of high energy states. But the entropy functionals and their behavior have an independent interest for the theory of orthogonal polynomials. We describe some results obtained in the last 15 years, as well as sketch the ideas behind their proofs.

1. Introduction

Given a probability density ρ, the expression $-\ln(\rho)$ is known as the *surprise level function*, whose mean value (average lack of information or uncertainty) is identified with the *Shannon entropy* of ρ [1]. In particular, if $\{\rho_j\}_{j=1}^n$ is a discrete probability distribution ($\rho_j \geq 0, \sum \rho_j = 1$), the information entropy functional

$$s_n := -\sum_{j=1}^{n} \rho_j \ln(\rho_j) \tag{1}$$

measures, in common perception, the uncertainty associated with this probability distribution. Two extremal cases are

$$\text{Uniform distribution: } \{\rho_j\}_{j=1}^n = \left\{\frac{1}{n}, \dots, \frac{1}{n}\right\} \quad \Rightarrow \quad s_n = \ln(n),$$
$$\text{Dirac delta: } \{\rho_j\}_{j=1}^n = \{0, \dots, 0, 1, 0, \dots, 0\} \quad \Rightarrow \quad s_n = 0.$$

Jensen's inequality applied to (1) gives

$$0 \leq s_n \leq \ln(n),$$

showing that the uniform distribution, having the most uncertain outcome, has maximal entropy, while the deterministic event has the minimal one.

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If ρ is a continuous probability distribution,

$$\rho(x) \geqslant 0, \quad x \in \mathbb{R}, \qquad \int_{\mathbb{R}} \rho(x)\mathrm{d}x = 1,$$

we can define by analogy the information entropy [1]

$$S_\rho = -\int \rho(x) \ln \rho(x) \mathrm{d}x, \tag{2}$$

known also as the *Boltzmann*, *Boltzmann–Shannon* or *differential* entropy, that characterizes the localization of the density of the distribution. The measures of information (1) and (2), although formally similar, have different properties. In particular, if ρ is a continuous probability distribution on $[a, b]$ and we introduce a discrete distribution

$$\rho_j = \int_{a+(j-1)h}^{a+jh} \rho(x)\mathrm{d}x, \quad j = 1, \ldots, n, h = (b-a)/n,$$

then $S_\rho \approx s_\rho + \ln(h)$, showing in particular that S_ρ is unbounded. In this sense, it is more convenient to consider an entropy functional for two (probability) measures, μ and ν,

$$\mathcal{K}(\mu, \nu) = \begin{cases} -\int \ln\left(\dfrac{\mathrm{d}\nu}{\mathrm{d}\mu}\right) \mathrm{d}\nu, & \text{if } \nu \text{ is } \mu\text{-a.c.,} \\ -\infty, & \text{otherwise.} \end{cases} \tag{3}$$

This is the *Kullback–Leibler information*, also known as the *relative* or *mutual* entropy, which measures the "distance" between ν and μ. Obviously, if ν is μ-a.c., we can also rewrite it as

$$\mathcal{K}(\mu, \nu) = -\int \frac{\mathrm{d}\nu}{\mathrm{d}\mu} \ln\left(\frac{\mathrm{d}\nu}{\mathrm{d}\mu}\right) \mathrm{d}\mu.$$

There is no a priori preferred notion of information measure in physical applications, but a relevant role played by the Boltzmann–Shannon entropy in quantum mechanics (and in particular, in the modern density functional theory [2]) is motivated in part by the entropic formulation of the uncertainty principle. Consider for instance a single particle system in D dimensions. For any quantum mechanical state the distribution density is $\rho(x) := |\Psi(x)|^2$, where $\Psi(x)$ is the corresponding wave function or physical solution of the associated Schrodinger equation. If γ is the distribution density in the momentum space, then the Heisenberg's uncertainty principle for the quantum mechanical system is a consequence of the following inequality (see [3,4]):

$$S_\rho + S_\gamma \geqslant D(1 + \ln \pi).$$

For the fundamental quantum mechanical systems (harmonic oscillator, hydrogen atom) the relevant component of the probability density of physical states are expressed by means of orthogonal polynomials (Gegenbauer, Laguerre, Hermite). This brought up the study of the entropy functionals for orthogonal polynomials (see [5] as well as the survey [6]).

Let μ be a positive unit Borel measure on $\mathbb{R}$ and let

$$p_n(x) = \kappa_n \prod_{j=1}^{n} \left(x - \zeta_j^{(n)}\right), \quad \kappa_n > 0, \quad n \in \mathbb{N}_0 := \mathbb{N} \cup \{0\}, \tag{4}$$

denote the corresponding sequence of *orthonormal* polynomials such that

$$\int p_n(x) p_m(x) \mathrm{d}\mu(x) = \delta_{mn}, \quad m, n \in \mathbb{N}_0.$$

Then we can define the sequence of probability measures ν_n, absolutely continuous with respect to μ, given by

$$\mathrm{d}\nu_n(x) = p_n^2(x)\mathrm{d}\mu(x), \quad n \in \mathbb{N}_0, \tag{5}$$

(note that $\nu_0 = \mu$). These measures are usually related with the quantum-mechanical probability distribution of physical states, and are standard objects of study in the analytic theory of orthogonal polynomials. As it was shown in [7], ν_n is associated with the behavior of the ratio p_{n+1}/p_n as $n \to \infty$.

The relative entropy

$$E_n := \mathcal{K}(\mu, \nu_n) = -\int p_n^2(x) \ln\bigl(p_n^2(x)\bigr) \mathrm{d}\mu(x) \tag{6}$$

is called the (continuous) information *entropy of orthogonal polynomials* $\{p_n\}$. Obviously, this is not the only way to define an entropy associated with orthogonal polynomials (4). For instance, for $j \in \{1, \ldots, n\}$, let

$$\psi_i = \ell_n(\zeta_j^{(n)})\, p_{i-1}^2(\zeta_j^{(n)}), \quad i = 1, \ldots, n,$$