The asymptotical spectrum of Jacobi matrices

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ABSTRACT

A method to calculate the asymptotical eigenvalue density (asymptotical density of zeros) $\rho(x)$ of Jacobi matrices (orthogonal polynomials) in terms of its moments is presented. This method does not require the convergence of continued fractions and inversion of functional transformations as previous ones do. It is shown to be applicable to a wide family of Jacobi matrices (orthogonal polynomials). As a byproduct the density $\rho(x)$ is explicitly found for certain classical orthogonal polynomials.

1. INTRODUCTION

Let $h_{ii} = a_i$ and $h_{i,i+1} = h_{i+1,i} = b_i$ be the matrix elements of a Jacobi matrix H, i.e. a real and symmetric tridiagonal matrix of dimension N. The problem of determining the asymptotical eigenvalue density (AED in short notation) $\rho(x)$ of a Jacobi matrix in terms of its components has been often present in different branches of physics and mathematics. To our knowledge only Dyson [1] for Jacobi matrices with $a_i = 0$ and Dean [2] succeed to give a method for calculating $\rho(x)$. This method which requires the convergence of a certain continued fraction and the inversion of a functional transformation presents however many problems for practical purposes. Moreover it can only be applied for those Jacobi matrices which fulfil certain restrictive conditions, e.g. if the a_i are positive, they must satisfy the following inequality :

$$4b_k^2 \leqslant a_k a_{k+1} \; ; \quad k = i, i+1, i+2, \ldots \; ; \quad i = 1, 2, \ldots \tag{1}$$

Here the author proposes an alternative method of calculating the AED $\rho(x)$ of any Jacobi matrix and applies it to a practical case which cannot be solved by Dean's method. This case corresponds to the Jacobi matrices defined as follows :

$$\begin{cases} a_m = \beta m^\Theta & \alpha \geqslant 0; \Theta \geqslant 0; \beta \text{ real number} \\ b_m = m^\alpha & m = 1, 2, 3, \ldots, N \end{cases} \tag{2}$$

One can observe that condition (1) is not fulfilled for each set of values (α, β, Θ). These matrices appear for different values (α, β, Θ) in certain physical contexts, see for instance [3] and references therein. On the other hand it is known that the characteristic polynomial $P_r(x)$ of the r-squared principal submatrices of a Jacobi matrix H forms a family of orthogonal polynomials $\{P_r(x); r = 1, 2, 3, \ldots\}$ which satisfy the following three-term recurrence relation :

$$\begin{aligned} &P_{m+1}(x) = (x - a_{m+1}) P_m(x) - b_m^2 P_{m-1}(x) \\ &P_o(x) = 1; \; P_1(x) = x - a_1 \\ &m = 1, 2, 3, \ldots \end{aligned} \tag{3}$$

Moreover the eigenvalues of a N-dimensional Jacobi matrix are the roots of the polynomial $P_N(x)$. Then it is naturally observed that the asymptotical $(N \to \infty)$ eigenvalue density of the matrix H defined by (2) is equal to the asymptotical root density of the corresponding family $\{P_r(x)\}$. To each set (α, β, Θ) there exists a family of orthogonal polynomials. In particular we could obtain certain classical orthogonal polynomials (Chebyshev, Hermite, ...) [5]. Therefore by calculating the AED of the Jacobi matrices defined by (2) one gets as a particular case the asymptotical density of zeros of certain classical orthogonal polynomials.

2. METHOD

We shall characterize the asymptotical eigenvalue density distribution $\rho(x)$ of a finite Jacobi matrix H by the knowledge of all its moments μ'_r, i.e.

$$\mu'_r = \int_c^d x^r \rho(x)\, dx \qquad r = 0, 1, 2, 3, \ldots$$

(c, d) being the support interval of $\rho(x)$. The quantities μ'_r are calculated by the following relation

$$\mu'_r = \lim_{N\to\infty} \mu'^{(N)}_r \qquad r = 0, 1, 2, 3, \ldots \tag{4}$$

which simply expresses the fact that μ'_r are the asymptotical limit of the corresponding moments $\mu'^{(N)}_r$ of the eigenvalue density $\rho^{(N)}(x)$ of the N-dimensional

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Jacobi matrix. The quantities $\mu_r'^{(N)}$ can be expressed [6] in terms of the matrix elements in the following compact form :

$$\mu_m'^{(N)} = \frac{1}{N} \sum_{(m)} F(r_1', r_1, r_2', r_2, \ldots, r_j', r_j, r_{j+1}') \sum_{i=1}^{N-x} a_i^{r_1'} \, b_i^{2r_1} \, a_{i+1}^{r_2'} \cdots a_{i+j-1}^{r_j'} \, b_{i+j-1}^{2r_j} \, a_{i+j}^{r_{j+1}'} \tag{5}$$

$$m = 1, 2, 3, \ \ldots, N$$

the first summation extending over all the partitions $(r_1', r_1, r_2', \ldots, r_j', r_j, r_{j+1}')$ of the number m, subject to the following condition

$$r_1' + r_2' + \ldots + r_{j+1}' + 2\,(r_1 + r_2 + \ldots + r_j) = m \tag{5a}$$

and such that if $r_s = 0$, $1 < s < j$, then r_k and r_k' are zero for each $k > s$. In the second summation, x denotes the number of non-vanishing r_i which take part in the corresponding partition of m. Besides, j takes the values m/2 or $\frac{m-1}{2}$ if m is even or odd respectively.

The coefficients F are defined as follows :

$$F(r_1', r_1, r_2', r_2, \ldots, r_{j-1}', r_{j-1}, r_j') = m \frac{(r_1' + r_1 - 1)!}{r_1'!\, r_1!} \cdot \frac{(r_1 + r_2' + r_2 - 1)!}{(r_1 - 1)!\, r_2'!\, r_2!} \cdot \frac{(r_2 + r_3' + r_3 - 1)!}{(r_2 - 1)!\, r_3'!\, r_3!} \cdot \ldots \cdot \frac{(r_{j-2} + r_{j-1}' + r_{j-1} - 1)!}{(r_{j-2} - 1)!\, r_{j-1}'!\, r_{j-1}!} \cdot \frac{(r_{j-1} + r_j' - 1)!}{(r_{j-1} - 1)!\, r_j'!} \tag{5b}$$

For the evaluation of these coefficients, we must take into account the following convention :

$$F(r_1', r_1, r_2', r_2, \ldots, r_{j-1}', 0, 0) = F(r_1', r_1, r_2', r_2, \ldots, r_{j-1}').$$

The first four moments (m = 1, 2, 3, 4) are explicitly written in terms of the matrix elements in [6].

3. APPLICATION

Let us consider the Jacobi matrix defined by (2). The moments $\mu_r'^{(N)}$ of its eigenvalue density take the following form according to (5) :

$$\mu_m'^{(N)} = \frac{1}{N} \sum_{(m)} F(r_1', r_1, r_2', \ldots, r_j, r_{j+1}') \beta^{r_1' + r_2' + \ldots + r_{j+1}'} \cdot \sum_{i=1}^{N-x} i^{\Theta r_1' + 2\alpha r_1} (i+1)^{\Theta r_2' + 2\alpha r_2} \cdots (i+j-1)^{\Theta r_j' + 2\alpha r_j} \cdots (i+j)^{\Theta r_{j+1}'}$$

Applying (4) we get for the moments of the AED :

$$\mu_m' = \sum_{(m)} F(r_1', r_1, r_2', \ldots, r_j, r_{j+1}') \beta^{r_1' + r_2' + \ldots + r_{j+1}'} \lim_{N \to \infty} \frac{1}{N} \sum_{i=1}^{N-x} i^{\Theta r_1' + 2\alpha r_1} \cdots (i+j)^{\Theta r_{j+1}'}$$

Using the binomial theorem and the following relation (See [7] pp. 122-124), valid for any positive q,

$$\sum_{k=1}^{n} k^q = \frac{n^{q+1}}{q+1} + 0\,(n^q) \tag{5c}$$

(where $B_2, B_4, \ldots$ are the Bernoulli numbers), we can get

$$\mu_m' = \sum_{(m)} F(r_1', r_1, r_2', \ldots, r_j, r_{j+1}') \beta^{r_1' + r_2' + \ldots + r_{j+1}'} \lim_{N \to \infty} \left\{ \frac{N^q}{q+1} + A_1 N^{q-1} + A_2 N^{q-2} + \ldots \right\} \tag{6}$$

q being defined for convenience as follows :

$$q = \Theta\,(r_1' + r_2' + \ldots + r_{j+1}') + 2\alpha\,(r_1 + r_2 + \ldots + r_j) \tag{7}$$

or, by using (5a),

$$q = m\alpha + (\Theta - \alpha)\,(r_1' + r_2' + \ldots + r_{j+1}')$$

$A_1, A_2, A_3, \ldots$ are functions of q, r_i, r_{i+1}, Θ, α and the Bernoulli numbers.

In order to get convergence for the moments μ_m' in (6), we choose an appropriate scale of eigenvalues. Such a choice depends on the maximum value q_{max} of q. According to (7) we distinguish three cases :

1. $\Theta > \alpha$. The value $q_{max} = m\Theta$ for $r_1' + r_2' + \ldots + r_{j+1}' = m$
2. $\Theta = \alpha$; $q = m\alpha$
3. $\Theta < \alpha$. The value $q_{max} = m\alpha$ for $r_1' + r_2' + \ldots + r_{j+1}' = 0$

We study separately the corresponding three possibilities of matrices (2).

Case 1 : $\Theta > \alpha$

Taking into account that the simplest partition $[r_1', r_1, r_2', r_2, \ldots, r_j, r_{j+1}']$ of m is $[m, 0, 0, 0, \ldots, 0, 0]$ and on the other hand that m is the maximum value of the sum $r_1' + r_2' + \ldots + r_{j+1}'$, we can write equation (6) as follows :

$$\mu_m' = F\,(m, 0, 0, 0, \ldots, 0, 0)\, \beta^m \lim_{N \to \infty} \frac{N^{m\Theta}}{m\Theta + 1} + F\,(m-2, 1, 0, 0, \ldots, 0, 0) \beta^{m-2} \lim_{N \to \infty} \frac{N^{(m-2)\Theta + 2\alpha}}{(m-2)\Theta + 2\alpha + 1}$$

$$+ F(m-3,1,1,0,\dots,0,0)\beta^{m-2} \lim_{N\to\infty} \frac{N^{(m-2)\Theta+2\alpha}}{(m-2)\Theta+2\alpha+1}$$

$$+ F(m-4,2,0,0,\dots,0,0)\beta^{m-4} \lim_{N\to\infty} \frac{N^{(m-4)\Theta+4\alpha}}{(m-4)\Theta+4\alpha+1}$$

$$+ \dots \tag{8}$$

We get all the moments μ'_m finite in the units $x(\beta N^{\Theta})^{-1}$. More precisely, eq. (8) shows that the moments of the AED $\rho(x/\beta N^{\Theta})$Jacobi matrix with $\Theta > \alpha$ take the form :

$$\mu'_m = \frac{1}{m\Theta+1} \qquad m = 1, 2, 3, \dots \tag{9}$$

It is often more convenient to know the central moments μ_m or moments about the mean, which can be calculated [9] from μ'_m as follows :

$$\mu_r = \sum_{m=0}^{r} (-\mu'_1)^{r-m} \binom{r}{m} \mu'_m \tag{10}$$

From (9) and (10) we get the central moments

$$\mu_r = \frac{1}{(\Theta+1)^r} \sum_{m=0}^{r} (-1)^{r-m} \binom{r}{m} \frac{(\Theta+1)^m}{m\Theta+1} \tag{11}$$

$$r = 1, 2, 3, \dots$$

In particular when $\Theta=1$ this expression is reduced to :

$$\mu_r = \begin{cases} 0 & \text{if } r \text{ odd} \\ \dfrac{1}{2^r(r+1)} & \text{if } r \text{ even} \end{cases}$$

which are the central moments of the so-called uniform or rectangular distribution $\rho(x/\beta N)=1$ defined in the interval $(-1/2, +1/2)$. In general [8], the knowledge of all the moments of a distribution does not determine it uniquely. (In our case however the uniqueness is fulfilled as we shall see later on.)
Moreover it is not easy to know the shape of the distribution from its moments. In this case it is useful to calculate the skewness γ_1 and excess or kurtosis γ_2 of the distribution which supply an approximate aspect of the distribution about its mean. From (11) we get

$$\gamma_1 = \frac{\mu_3}{\mu_2^{3/2}} = \frac{2(\Theta-1)(2\Theta+1)^{1/2}}{3\Theta+1} \tag{12a}$$

$$\gamma_2 = \frac{\mu_4}{\mu_2^2} - 3 = \frac{6(2\Theta^3 - 6\Theta^2 - \Theta + 1)}{(3\Theta+1)(4\Theta+1)} \tag{12b}$$

One can observe that γ_1 only vanishes for a non-negative Θ, namely $\Theta = 1$.
Therefore the only possibility for the eigenvalues of the matrix (2) with $\Theta > \alpha$ to be symmetrically distributed is the rectangular distribution, and this happens when $\Theta = 1$ as we have seen above.

Case 2 : $\Theta = \alpha$

In this case $q = m\alpha$. From (6) we can then obtain that

$$\mu'_m = \frac{1}{m\alpha+1} \sum_{(m)} F(r'_1, r_1, r'_2, r_2, \dots, r_j, r'_{j+1}) \beta^{r'_1 + r'_2 + \dots + r'_{j+1}} \tag{13}$$

(where j is m/2 for m even and (m-1)/2 for m odd) are the moments of the AED $\rho(x/N^{\alpha})$ of the Jacobi matrix (2) with $\Theta=\alpha$. By using the properties (5b) of the coefficients F, eq. (13) is reduced to the following form :

$$\mu'_m = \frac{1}{m\alpha+1} \sum_{i=0}^{j} \binom{m}{2i} \binom{2i}{i} \beta^{m-2i} \tag{14}$$

They are also the moments of the asymptotical eigenvalue density of the orthogonal polynomials defined by the following recurrence relation :

$$P_{m+1}(x) = [x - \beta(m+1)^{\alpha}] P_m(x) - m^{2\alpha} P_{m-1}(x)$$

$$P_0(x) = 1; \; P_1(x) = x - \beta; \; m = 1, 2, 3, \dots \tag{15}$$

In particular when $\beta=0$, expression (14) can be written as follows :

$$\begin{cases} \mu'_{2k} = \dfrac{1}{2k\alpha+1} \dbinom{2k}{k} \\ \mu'_{2k-1} = 0 \end{cases} \qquad k = 1, 2, 3, \dots \tag{16}$$

If now $\alpha=0$, the moments (16) are those of the density distribution $\rho(x) = (1/\pi)(4-x^2)^{-1/2}$. Therefore the asymptotical root distribution of the orthogonal polynomials (15) with $\beta=\alpha=0$ (this is the case of Chebyshev polynomials) is the inverse of a semicircle whose support interval is $(-2, +2)$. Furthermore one can easily verify that the eigenvalues of the orthogonal polynomials defined by

$$P_{m+1}(x) = x P_m(x) - \xi P_{m-1}(x)$$

$$P_0(x) = 1; P_1(x) = x; \; \xi > 0; \; m = 1, 2, 3, \dots$$

are distributed asymptotically by the function

$\rho(x) = \frac{\sqrt{\xi}}{\pi} (4\xi - x^2)^{-1/2}$ on the interval $(-2\sqrt{\xi}, +2\sqrt{\xi})$.

On the other hand equation (16) for $\alpha=1/2$ shows the moments of the distribution $y=(1/2\pi)(4-z^2)^{1/2}$. Therefore for large N it is found that the distribution of the zeros of the orthogonal polynomials (15) with $\beta=0$ and $\alpha=1/2$ (this is the case of Hermite polynomials) is given by $\rho(x)=(1/2\pi\sqrt{N})(4N-x^2)^{1/2}$ in the interval $(-2\sqrt{N}, +2\sqrt{N})$.
From (14) we can get the skewness γ_1 and excess γ_2 of the corresponding density distribution. Their explicit expressions in terms of α and β are complicated and are not written here. However it is interesting to say that only if $\alpha = (1+\sqrt{2})/2$ and $\beta = 0$ the values γ_1

and γ_2 vanish simultaneously. For this pair of values (α, β), the moments of the AED are given by

$$\mu_{2k} = \frac{1}{k(1+\sqrt{2})+1} \binom{2k}{k} \qquad k = 1, 2, 3, \ldots$$

$$\mu_{2k-1} = 0$$

which correspond to a quasi-Gaussian distribution, that is a distribution very close to the normal one.

Case 3 : $\Theta < \alpha$

Now $q_{max} = m\alpha$, which corresponds to the partition $[0, r_1, 0, r_2, \ldots, 0, r_j, 0]$ of m. From (6) one can observe that all the moments μ'_m do not diverge if one takes $xN^{-\alpha}$ as eigenvalue variable. With this choice, expression (6) reduces as follows :

$$\mu'_m = \frac{1}{m\alpha+1} \sum_{(m)} F(0, r_1, 0, r_2, \ldots, 0, r_j, 0)$$

with $r_1 + r_2 + \ldots + r_j = \frac{m}{2}$

Using the properties of the coefficients F, we can get:

$$\mu'_{2k} = \frac{1}{2k\alpha+1} \binom{2k}{k} \qquad k = 1, 2, 3, \ldots$$

$$\mu'_{2k-1} = 0 \tag{17}$$

which are the moments of the AED $\rho(xN^{-\alpha})$ of the Jacobi matrices (2) with $\alpha > \Theta$. Equally well one can say that the AED $\rho(xN^{-\alpha})$ of the orthogonal polynomials defined by

$$P_{m+1}(x) = [x - \beta(m+1)^{\Theta}] P_m(x) - m^{2\alpha} P_{m-1}(x)$$

$$P_0(x) = 1; \; P_1(x) = x - \beta; \; \alpha > \Theta; \; m = 1, 2, 3, \ldots \tag{18}$$

have the moments given by (17). This result was already found for $\beta = 0$ in equation (16) above, since for such value of β the polynomials (15) and (18) are the same.
In addition one can observe that not only the Hermite polynomials (which require $\beta = 0$ and $\alpha = \Theta = 1/2$ as we have seen above) but all the polynomials (18) with $\alpha = 1/2$ and $\Theta < 1/2$ have

$$\rho(x) = (1/2\pi\sqrt{N})\,(4N - x^2)^{1/2}$$

as the distribution of zeros for large N.
Thus far, the moments of all orders of the AED $\rho(x)$ of the Jacobi matrices (2) have been calculated and at times the analytical expression $\rho(x)$ is obtained. In general to calculate the function $\rho(x)$ from its moments it is necessary [9] to sum the series

$$\Psi(t) = \sum_{k=0}^{\infty} \frac{\mu'_k}{k!} (it)^k \tag{19}$$

and then to do the following transformation :

$$\rho(x) = \int_{-\infty}^{+\infty} e^{-itx}\, \Psi(t)\, dt$$

However this way of getting $\rho(x)$ is not useful when the power series (19) slowly converges except for small t.
Finally it is known [9, 10] that the moments do not always determine completely a distribution, even when moments of all orders exist. Only when the support interval (a, b) is finite, the knowledge of all the moments uniquely determines the distribution. When (a, b) is equal to $(-\infty, +\infty)$ or $(0, +\infty)$ only some sufficient conditions for $\rho(x)$ to be unique are known; perhaps the most useful one (see [8], Corollary 1.2, pag. 20) is that $\rho(x)$ decrease exponentially or faster for large $|x|$, or equivalently that μ'_r grows no faster than r! for large r. It can be easily seen that the moments (9), (14) and (17) fulfil this condition. Therefore they determine uniquely $\rho(x)$ for any interval (a, b).

4. CONCLUSION

A method for calculating the eigenvalue density of a Jacobi matrix H with elements $h_{ii} = a_i$ and $h_{i,i+1} = h_{i+1,i} = b_i$, or equivalently the density of zeros of the orthogonal polynomials defined by (3), has been proposed. It has been shown to be applicable to a broad family of Jacobi matrices (orthogonal polynomials). As a particular case the asymptotical density of zeros of Chebyshev and Hermite polynomials has been found.

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The author would like to acknowledge the hospitality extended to him by Prof. Amand Faessler at the Kernforschungsanlage Jülich.

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