Advances in Applied Mathematics and Mechanics
Adv. Appl. Math. Mech., Vol. **8**, No. 1, pp. 117-127

DOI: 10.4208/aamm.2014.m504
February 2016

On Polynomial Maximum Entropy Method for Classical Moment Problem

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Received 12 February 2014; Accepted (in revised version) 15 December 2014

Abstract. The maximum entropy method for the Hausdorff moment problem suffers from ill conditioning as it uses monomial basis $\{1,x,x^2,\cdots,x^n\}$. The maximum entropy method for the Chebyshev moment probelm was studied to overcome this drawback in [4]. In this paper we review and modify the maximum entropy method for the Hausdorff and Chebyshev moment problems studied in [4] and present the maximum entropy method for the Legendre moment problem. We also give the algorithms of converting the Hausdorff moments into the Chebyshev and Lengendre moments, respectively, and utilizing the corresponding maximum entropy method.

AMS subject classifications: 41A35, 65D07, 65J10

Key words: Classical moment problem, monomials, Chebyshev polynomials, Legendre polynomials.

1 Introduction

The *Hausdorff moment problem* is to find an unknown density f^* such that

$$\int_0^1 f^*(x)x^i dx = \mu_i, \quad i=0,1,2,\cdots.$$

It is well known [11] that the above problem has a solution if and only if the moment sequence $\{\mu_i\}$ is *positive definite*, i.e., $\Delta^m \mu_i \geq 0$ for all m and i, where Δ^m is the m-th forward difference.

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Many mathematical physics problems are equivalent to the moment problem. Practically, it is often the case that only a finitely many moments are available. Thus, it is desired to determine a density f that satisfies all the known moment conditions

$$\int_0^1 f(x)x^i dx = \mu_i, \quad i=0,1,2,\cdots,n.$$

Mathematically there are infinitely many candidates for the required function, so how to locate the *best one* among them is important in applications.

The maximum entropy principle provides the most unbiased criterion for choosing the best candidate with the given moments. In other words, the determined density function gives the maximum entropy among all the densities with the given moments. The realization of this principle is the solution of the following optimization problem: maximize

$$H(f) = -\int_0^1 f(x)\ln f(x)dx$$

among all the density functions subject to

$$\int_0^1 f(x)x^i dx = \mu_i, \quad i=0,1,2,\cdots,n.$$

Here the objective function H is called the *Boltzmann* entropy.

This principle was first proposed by Jayne in 1957 to numerically recover an unknown density function in mathematical physics [8]. The resulting numerical scheme is well known now as the maximum entropy method [10], and its idea has been extended to solving, for example, Frobenius-Perron operator equations [1,2,4–6] for the computation of a stationary density of an interval mapping $S:[0,1]\to[0,1]$.

Although it is widely useful in physical science and engineering [3, 10], the classical maximum entropy method using Hausdorff moments has an intrinsic drawback of sensitivity issue. Namely, the resulting system of nonlinear equations from the above constrained maximization problem is ill-conditioned due to the involvement of the standard monomial basis $\{1,x,x^2,\cdots,x^n\}$. So in [4] to overcome this drawback Chebyshev polynomial basis was used.

In this paper we review and modify the Hausdorff and Chebyshev maximum entropy methods and study Legendre maximum entropy method. We also consider the algorithms of converting the Hausdorff moments into the Chebyshev and Legendre moments, respectively, and solving the corresponding moment problems with the maximum entropy method.

We briefly review the basic properties of the Chebyshev and Legendre polynomials in the next section. Then we review the general maximum entropy method in Section 3. In Section 4 we develop a polynomial maximum entropy method. Then in Section 5 we consider the algorithms of converting the Hausdorff moments into the Chebyshev or Legendre moments. Numerical experiments of all the algorithms discussed in the paper are performed and compared in Section 6. We conclude in Section 7.

2 Chebyshev and Legendre polynomials

Let ω be a nonnegative function defined on an open interval (a,b). A sequence of polynomials p_n is said to be orthogonal with respect to the weight function ω over $[a,b]$ if

$$\langle p_i,p_j\rangle := \int_a^b p_i(x)p_j(x)\omega(x)dx = 0,$$

whenever $i \neq j$. For example, the Chebyshev polynomials

$$T_i(x) = \cos(i\arccos x), \quad i = 0,1,\cdots,$$

are orthogonal polynomials with respect to $\omega(x) = 1/\sqrt{1-x^2}$ over the interval $[-1,1]$. It is well known that the Chebyshev polynomials satisfy the following recursive formula

$$T_i(x) = 2xT_{i-1}(x) - T_{i-2}(x), \quad i = 2,3,\cdots, \tag{2.1}$$

with $T_0(x) = 1$ and $T_1(x) = x$.

Similarly, the Legendre polynomials can be generated by the recursive formula

$$L_i(x) = \frac{2i-1}{i}xL_{i-1}(x) - \frac{i-1}{i}L_{i-2}(x), \quad i = 2,3,\cdots, \tag{2.2}$$

with $L_0(x)=1$ and $L_1(x)=x$, and they are orthogonal polynomials with respect to $\omega(x)=1$ over the interval $[-1,1]$. The first four Chebyshev polynomials are

$$T_0(x) = 1, \quad T_1(x) = x, \quad T_2(x) = 2x^2 - 1, \quad T_3(x) = 4x^3 - 3x,$$

and the corresponding Legendre polynomials are

$$L_0(x) = 1, \quad L_1(x) = x, \quad L_2(x) = \frac{3}{2}x^2 - \frac{1}{2}, \quad L_3(x) = \frac{5}{2}x^3 - \frac{3}{2}x.$$

In general, T_i and L_i are even functions if i is even, and odd functions if i is odd. We also note that if $\{p_i\}$ is a sequence of orthogonal polynomials with respect to the weight function ω over $[a,b]$, then $\{p_i((b-a)x+a)\}$ is an orthogonal polynomial sequence with respect to the weight function $\omega((b-a)x+a)$ over $[0,1]$.

3 Maximum entropy approach to moment problem

Let $L^1(0,1)$ be the space of all Lebesgue integrable functions defined on $[0,1]$, and denote by D the set of all density functions, i.e., a nonnegative functions in $L^1(0,1)$ with integral value 1.

In the maximum entropy method for numerically approximating an unknown density function f^* satisfying

$$\int_0^1 f^*(x)g_i(x)dx = \mu_i, \quad i = 0,1,\cdots,n, \tag{3.1}$$

one maximizes the *Boltzmann entropy functional H* defined by

$$H(f) = -\int_0^1 f(x)\ln f(x)dx, \quad f \in D,$$

with the equality constraints

$$\int_0^1 f(x)g_i(x)dx = \mu_i, \quad i = 0,1,\cdots,n,$$

where $g_0,g_1,\cdots,g_n \in L^\infty(0,1)$. These functions $g_0,g_1,\cdots,g_n$ are called the *moment functions*.

It is well known [9] that the maximum entropy solution to the above constrained maximization problem exists and is unique. In fact, it has an explicit expression of the form

$$f_n(x) = \frac{\exp\left(\sum_{j=0}^n \lambda_j g_j(x)\right)}{\int_0^1 \exp\left(\sum_{j=0}^n \lambda_j g_j(x)\right)dx},$$

where the numbers $\lambda_0,\lambda_1,\cdots,\lambda_n$ are chosen to satisfy the given constraints

$$\int_0^1 f_n(x)g_i(x)dx = \mu_i, \quad i = 0,1,\cdots,n.$$

4 Polynomial maximum entropy method

First of all, we review the polynomial maximum entropy method developed in [4]. Suppose that we choose the moment functions $g_i(x) = x^i$ for $i = 0,1,\cdots,n$. Then the corresponding f_n is written as

$$f_n(x) = \frac{\exp\left(\sum_{j=0}^n \lambda_j x^j\right)}{\int_0^1 \exp\left(\sum_{j=0}^n \lambda_j x^j\right)dx},$$

where the numbers $\lambda_0,\lambda_1,\cdots,\lambda_n$ are chosen to satisfy the given constraints

$$\int_0^1 f_n(x)x^i dx = \mu_i, \quad i = 0,1,\cdots,n.$$

Note that using

$$\exp\Big(\sum_{j=0}^n \lambda_j x^j\Big) = e^{\lambda_0}\exp\Big(\sum_{j=1}^n \lambda_j x^j\Big),$$

we have

$$f_n(x) = \frac{\exp\left(\sum_{j=1}^n \lambda_j x^j\right)}{\int_0^1 \exp(\sum_{j=1}^n \lambda_j x^j)dx}.$$

So the corresponding constraints become

$$\frac{\int_0^1 \exp\big(\sum_{j=1}^n \lambda_j x^j\big) x^i dx}{\int_0^1 \exp\big(\sum_{j=1}^n \lambda_j x^j\big) dx} = \mu_i, \quad i=0,1,\cdots,n.$$

Since f^* is a density and $g_0 = x^0 = 1$, it follows from (3.1) that $\mu_0 = 1$. Thus in the above constraints the equation corresponding to $i=0$ is automatically fulfilled for any $\lambda_1,\cdots,\lambda_n$. Hence we have come up with the following form of f_n

$$f_n(x) = \frac{\exp\big(\sum_{j=1}^n \lambda_j x^j\big)}{\int_0^1 \exp\big(\sum_{j=1}^n \lambda_j x^j\big) dx}$$

and the corresponding constraints

$$\frac{\int_0^1 \exp\big(\sum_{i=1}^n \lambda_j x^j\big) x^i dx}{\int_0^1 \exp\big(\sum_{j=1}^n \lambda_j x^j\big) dx} = \mu_i, \quad i=1,\cdots,n.$$

Based upon these equations, the Hausdorff maximum entropy algorithm was developed in [4]. Similarly, in [4] the Chebyshev maximum entropy algorithm was developed based upon

$$f_n(x) = \frac{\exp\big(\sum_{j=1}^n \lambda_j T_j(2x-1)\big)}{\int_0^1 \exp\big(\sum_{j=1}^n \lambda_j T_j(2x-1)\big) dx}$$

and

$$\frac{\int_0^1 \exp\big(\sum_{i=j}^n \lambda_j T_j(2x-1)\big) T_i(2x-1) dx}{\int_0^1 \exp\big(\sum_{j=1}^n \lambda_j T_j(2x-1)\big) dx} = \mu_i, \quad i=1,\cdots,n.$$

In this paper we modify these maximun entropy equations based on a simple observation which is presented in the following lemma.

Lemma 4.1. *Assume that* $1 \in \mathrm{span}\{g_0,g_1,\cdots,g_n\}$*. If* $\lambda_0,\lambda_1,\cdots,\lambda_n$ *satisfy*

$$\int_0^1 \exp\Big(\sum_{j=0}^n \lambda_j g_j(x)\Big) g_i(x) dx = \mu_i, \quad i=0,1,\cdots,n, \tag{4.1}$$

then the maximum entropy solution f_n *can be written as*

$$f_n(x) = \exp\Big(\sum_{j=0}^n \lambda_j g_j(x)\Big).$$

Proof. It is enough to show that $\exp(\sum_{j=0}^{n}\lambda_j g_j(x))$ is a density. Since 1 belongs to $\text{span}\{g_0,g_1,\cdots,g_n\}$, there exist some constants $c_0,c_1,\cdots,c_n$ such that $\sum_{i=0}^{n}c_i g_i(x)=1$. The fact that $f^*\in D$ and (3.1) lead to

$$\sum_{i=0}^{n}c_i\mu_i=\sum_{i=0}^{n}c_i\int_0^1 f^*(x)g_i(x)dx=\int_0^1 f^*(x)\sum_{i=0}^{n}c_i g_i(x)dx=\int_0^1 f^*(x)\cdot 1dx=1.$$

So using (4.1) yields

$$\begin{aligned}\int_0^1 \exp\Big(\sum_{j=0}^{n}\lambda_j g_j(x)\Big)dx&=\int_0^1 \exp\Big(\sum_{j=0}^{n}\lambda_j g_j(x)\Big)\sum_{i=0}^{n}c_i g_i(x)dx\\&=\sum_{i=0}^{n}c_i\int_0^1 \exp\Big(\sum_{j=0}^{n}\lambda_j g_j(x)\Big)g_i(x)dx=\sum_{i=0}^{n}c_i\mu_i=1.\end{aligned}$$

So, we complete the proof. □

Remark 4.1. In all of the Hausdorff, Chebyshev, and Legendre maximum entropy methods $g_0(x)=1$. So Lemma 4.1 applies to all of them.

Remark 4.2. The *partition of unity* property of the piecewise linear method in [2] is also a special case of Lemma 4.1 as 1 belongs to the span of the piecewise linear moment functions.

Assume that $1\in\text{span}\{g_0,g_1,\cdots,g_n\}$ and that

$$\mu_i=\int_0^1 f^*(x)g_i(x)dx,\quad i=0,1,\cdots,n,$$

are given. Now we want to approximate the density f^* with f_n. Then the corresponding maximum entropy method can be summarized as follows.

Step 1 Solve the following system of nonlinear equations

$$\int_0^1 \exp\Big(\sum_{j=0}^{n}\lambda_j g_j(x)\Big)g_i(x)dx=\mu_i,\quad i=0,1,\cdots,n,$$

for $\lambda_0,\lambda_1,\cdots,\lambda_n$.

Step 2 The maximum entropy solution is

$$f_n(x)=\exp\Big(\sum_{i=0}^{n}\lambda_i g_i(x)\Big).$$

Remark 4.3. If $g_i(x)=x^i$, we have the Hausdorff maximum entropy method; if $g_i(x)=T_i(2x-1)$, we have the Chebyshev maximum entropy method; and if $g_i(x)=L_i(2x-1)$, we have the Legendre maximum entropy method.

5 Converting Hausdorff moments into Chebyshev and Legendre moments

Because of high ill-conditioning of the Hausdorff moment problem solved directly with the maximum entropy method, converting the Hausdorff moment problem into an orthogonal polynomial moment problem is of practical importance in realizing the maximum entropy principle. Using the recursive formula (2.1) it is easy to figure out all the coefficients of $T_i(x)$ for any i. So write

$$T_i(x)=c_{i0}+c_{i1}x+\cdots+c_{ii}x^i.$$

Then we can compute $\tilde{c}_{ij}$, $0\le j\le i\le n$, such that

$$\begin{aligned}T_i(2x-1)&=c_{i0}+c_{i1}(2x-1)+\cdots+c_{ii}(2x-1)^i\\&=c_{i0}+c_{i1}(-1+2x)+\cdots+c_{ii}\sum_{j=0}^{i}\binom{i}{j}(-1)^{i-j}2^jx^j=\sum_{j=0}^{i}\tilde{c}_{ij}x^j.\end{aligned}$$

If we let $\mu\in\mathbf{R}^{n+1}$ with $\mu_i=\int_0^1 f^*(x)x^i dx$ for $i=0,1,\cdots,n$, and $\tilde{\mu}\in\mathbf{R}^{n+1}$ with $\tilde{\mu}_i=\int_0^1 f^*(x)T_i(2x-1)dx$ for $i=0,1,\cdots,n$, then

$$\tilde{\mu}_i=\int_0^1 f^*(x)T_i(2x-1)dx=\int_0^1 f^*(x)\sum_{j=0}^{i}\tilde{c}_{ij}x^jdx=\sum_{j=0}^{i}\tilde{c}_{ij}\int_0^1 f^*(x)x^jdx=\sum_{j=0}^{i}\tilde{c}_{ij}\mu_j,$$

for $i=0,1,\cdots,n$. So if we define the $(n+1)\times(n+1)$ lower triangular matrix $\tilde{M}$ whose (i,j)-entry is $\tilde{c}_{ij}$ for $0\le j\le i\le n$, then

$$\tilde{\mu}=\tilde{M}\mu,$$

where $\tilde{\mu}$ is the vector of Chebyshev moments.

Similarly, using (2.2) we can find $\hat{c}_{ij}$, $0\le j\le i\le n$, such that

$$L_i(2x-1)=\sum_{j=0}^{i}\hat{c}_{ij}x^j.$$

Then, as before, if we define the $(n+1)\times(n+1)$ lower triangular matrix $\hat{M}$ whose (i,j)-entry is $\hat{c}_{ij}$ for $0\le j\le i\le n$, we have

$$\hat{\mu}=\hat{M}\mu,$$

where $\hat{\mu}$ is the vector of Legendre moments.

So we can use the Chebyshev or Legendre maximum entropy methods starting with the Housdorff moments to reduce the instability of the traditional maximum entropy approach. In the next section we present the numerical implementation results of these different schemes applied to solving the Frobenius-Perron fixed density equation.

6 Numerical results

We first introduce the concept of the Frobenius-Perron operator for one dimensional transformations. Let a measurable transformation $S:[0,1]\to[0,1]$ be nonsingular, that is, $m(A)=0$ implies $m(S^{-1}(A))=0$ for every Lebesgue measurable subset A of $[0,1]$, where m denotes the Lebesgue measure. The linear operator $P_S:L^1(0,1)\to L^1(0,1)$ defined by

$$\int_A P_S f(x)dx=\int_{S^{-1}(A)} f(x)dx$$

for every measurable $A\subset[0,1]$ is called the *Frobenius-Perron operator* associated with S. An extensive study of this class of Markov operators is referred to, e.g., [7,9].

In the applications of ergodic theory to physical and engineering problems, stationary density functions, which are also fixed points of Frobenius-Perron operators, play an important role since they determine the statistical properties of the deterministic dynamics of the corresponding transformation.

In this section we use several versions of the polynomial maximum entropy method to numerically recover a stationary density. We used the following piecewise monotonic interval mapping

$$S(x)=\begin{cases} \dfrac{2x}{1-x^2}, & 0\le x\le\sqrt{2}-1, \\ \dfrac{1-x^2}{2x}, & \sqrt{2}-1\le x\le 1, \end{cases}$$

to test the performance of the Hausdorff (H-MEM), Chebyshev (C-MEM) and Legendre (L-MEM) maximum entropy methods as well as the algorithms of converting the Haudroff moments to the Chebyshev (HC-MEM) and Legendre moments (HL-MEM) and applying the corresponding maximum entropy methods. The unique stationary density of S is positive and given by

$$f^*(x)=\frac{4}{\pi(1+x^2)}.$$

After we used Newton's method to solve the nonlinear system of equations for f_n, we estimated the L^1-norm error

$$e_n=\|f_n-f^*\|_1=\int_0^1|f_n(x)-f^*(x)|dx$$

with a numerical integration scheme. In Table 1, we recorded the L^1-norm errors with $n=1,2,\cdots,12$, using H-MEM, C-MEM, and L-MEM, and in Table 2, we recorded the maximum matrix 1-norm condition numbers of the derivative matrix encountered during Newton's iterations for each n. In Table 3, we recorded the L^1-norm errors with different

Table 1: L^1-norm errors in f_n.

n	H-MEM	C-MEM	L-MEM
1	3.3×10^{-2}	3.3×10^{-2}	3.3×10^{-2}
2	6.7×10^{-3}	6.7×10^{-3}	6.7×10^{-3}
3	2.1×10^{-4}	2.1×10^{-4}	2.1×10^{-4}
4	1.8×10^{-4}	1.8×10^{-4}	1.8×10^{-4}
5	3.0×10^{-5}	3.0×10^{-5}	3.0×10^{-5}
6	1.6×10^{-6}	1.6×10^{-6}	1.6×10^{-6}
7	1.3×10^{-6}	1.3×10^{-6}	1.3×10^{-6}
8	3.3×10^{-7}	1.6×10^{-7}	1.6×10^{-7}
9	2.0×10^{-4}	2.3×10^{-8}	2.3×10^{-8}
10	1.3×10^{-5}	9.8×10^{-9}	9.8×10^{-9}
11	2.4×10^{-7}	7.7×10^{-10}	7.7×10^{-10}
12	1.3×10^{-5}	2.7×10^{-10}	2.7×10^{-10}

Table 2: Maximum matrix 1-norm condition number encountered in computing f_n.

n	H-MEM	C-MEM	L-MEM
1	2.7×10^{1}	3.8×10^{0}	3.8×10^{0}
2	7.5×10^{2}	6.8×10^{0}	6.9×10^{0}
3	2.8×10^{4}	1.2×10^{1}	9.8×10^{0}
4	9.4×10^{5}	1.5×10^{1}	1.3×10^{1}
5	2.9×10^{7}	1.9×10^{1}	1.6×10^{1}
6	9.9×10^{8}	2.2×10^{1}	1.9×10^{1}
7	3.4×10^{10}	2.7×10^{1}	2.2×10^{1}
8	9.9×10^{11}	3.0×10^{1}	2.6×10^{1}
9	3.7×10^{15}	3.4×10^{1}	2.9×10^{1}
10	1.6×10^{14}	3.7×10^{1}	3.2×10^{1}
11	1.3×10^{13}	4.1×10^{1}	3.6×10^{1}
12	1.6×10^{14}	4.4×10^{1}	3.9×10^{1}

n using HC-MEM and HL-MEM, and in Table 4, we recorded the matrix 1-norm condition numbers of the conversion matrices $\tilde{M}$ and $\hat{M}$ respectively for each n.

From Table 1 we can see that both the Chebyshev and Legendre maximum entropy methods outperform the Hausforff maximum entropy method considerably, especially when the number of the moments becomes large since the errors of the latter do not decrease for those n due to the instability signaled by the high condition numbers which can be seen from Table 2. We also observe from Table 2 that the condition numbers for the orthogonal polynomial based maximum entropy methods are only in the order of 10^1 for all n in this example, as compared to the order of 10^{14} with $n=9,10,11,12$ for the Hausdorff maximum entropy method.

For the algorithms of converting the Hausdorff moments to the Chebyshev and Leg-

Table 3: L^1-norm errors in f_n.

n	HC-MEM	HL-MEM
1	3.3×10^{-2}	3.3×10^{-2}
2	6.7×10^{-3}	6.7×10^{-3}
3	2.1×10^{-4}	2.1×10^{-4}
4	1.8×10^{-4}	1.8×10^{-4}
5	3.0×10^{-5}	3.0×10^{-5}
6	1.6×10^{-6}	1.6×10^{-6}
7	1.3×10^{-6}	1.3×10^{-6}
8	1.6×10^{-7}	1.6×10^{-7}
9	2.4×10^{-8}	2.3×10^{-8}
10	9.8×10^{-9}	9.8×10^{-9}
11	2.5×10^{-9}	2.8×10^{-9}
12	2.1×10^{-8}	1.9×10^{-8}

Table 4: Matrix 1-norm condition numbers of $\tilde{M}$ and $\hat{M}$.

n	$\tilde{M}$	$\hat{M}$
1	3.0×10^{0}	3.0×10^{0}
2	1.9×10^{1}	1.5×10^{1}
3	1.2×10^{2}	7.5×10^{1}
4	7.1×10^{2}	3.7×10^{2}
5	3.8×10^{3}	1.8×10^{3}
6	2.4×10^{4}	1.0×10^{4}
7	1.4×10^{5}	5.5×10^{4}
8	8.3×10^{5}	3.0×10^{5}
9	5.1×10^{6}	1.7×10^{6}
10	3.2×10^{7}	1.0×10^{7}
11	1.9×10^{8}	5.5×10^{7}
12	1.1×10^{9}	3.1×10^{8}

endre moments, we see that the growing condition numbers of the conversion matrices (Table 4) limit the accuracy of the algorithms HC-MEM and HL-MEM (Table 3). However, the algorithms HC-MEM and HL-MEM are still more accurate that the algorithm H-MEM. So if only the Hausdorff moments are available, it is recommened to use the algorithms HC-MEM or HL-MEM rather than the algorithm H-MEM.

7 Conclusions

Using a very mild condition that the constant function 1 can be written as a linear combination of the moment functions used in the maximum entropy method, which is often the case in the numerical implementation of the method, such as the monomial moment functions, orthogonal polynomial moment functions, and piecewise polynomial moment functions satisfying the partition of unity property, we have been successful in removing the denominator in the nonlinear system of equations, thus simplied the algorithms. We have also demonstrated that an orthogonal maximum entropy method outpeform the monomial maximum entropy method. Finally, we discussed how to reduce the ill-conditioning of the monomial moment problem by converting the monomial moments into orthogonal polynomial moments.

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