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A generalization of the moment problem to a complex density and higher order approximations in the heat equation ⋆

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Abstract. The moment problem is about positive density functions and this positivity restriction makes its application to sign-changing functions limited. In this paper we generalize the moment problem to complex density functions. This extended theory allows us to work with an arbitrary real sequence by simply setting them as the real parts of complex moments. As an application we take the moments of sign-changing solutions of the heat equation at a backward time, say $t = -t_0$. Then the extended theory allows a construction of an approximation of the solution which consists of n summations of elementary functions. This approximation shows a geometric convergence as $n \to \infty$ and of convergence order $O(t^{\frac{1}{2p}-\frac{2n+1}{2}})$ in L^p-norm as $t \to \infty$. The use of the backward moments also gives a good approximation for $0 < t \ll 1$ small. Numerical examples that show several interesting properties are included.

1. Introduction

Let a sequence of real numbers $\alpha_k \in \boldsymbol{R}$, $0 \le k \le 2n-1$, be given. The one dimensional truncated moment problem related to this sequence is to find real ρ_i's and c_i's, $1 \le i \le n$, that satisfy

$$\sum_{i=1}^{n} \rho_i c_i^k = \alpha_k, \quad k = 0, 1, \cdots, 2n-1 \tag{1}$$

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(see, e.g., [4]). It is well known that, if the sequence α_k's are k-th order moments of a positive density function, there exist such ρ_i's and c_i's in a unique way.

However, if α_k's are moments of a sign-changing density, or taken arbitrary, then the existence and the uniqueness of the truncated moment problem are not guaranteed. Due to this positivity restriction its application has been limited. For example, the theory was applied to construct an approximation of higher order convergence for solutions to the heat equation in [15]. However, this asymptotic theory has been completed for positive solutions only and left incomplete for sign-changing solutions. The main purpose of this paper is to generalize the theory of moment problem to handle arbitrary sequences, and then show the applicability of this extended theory by completing the higher order approximation theory in the heat equation. This example convinces us that the generalization of the moment problem to complex density functions increase its applicability considerably.

This paper consists of two parts. One is for the generalization of the moment problem, and the other is for its application to the heat equation. Consider the approximation theory developed in [15] which exploits on the moments of the solution to the heat equation

$$u_t = u_{xx}, \quad u(x,0) = u_0(x), \qquad u, x \in \boldsymbol{R}, \tag{2}$$

where the initial value $u_0(x)$ is assumed to have finite moments up to $2n$-th order, i.e., $x^{2n}u_0(x) \in L^1(\boldsymbol{R})$. It is well known that the solution to the heat equation is given as

$$u(x,t) = \int u_0(c)\phi(x-c,t)dc, \quad x, c \in \boldsymbol{R}, \tag{3}$$

where ϕ is the heat kernel. This integration formula gives the exact value of the solution. However, one may do the integration only approximately and hence finding an efficient way to compute such an integration formula has been an important issue. Here, we find an approximation of the solution using elementary functions.

Let $\alpha_k(t)$ be the k-th order moments of the solution $u(x,t)$, i.e.,

$$\alpha_k(t) := \int_{-\infty}^{\infty} x^k u(x,t)dx, \qquad k = 0, 1, \cdots, 2n-1.$$

Note that, even if the solution $u(x,t)$ is not defined for a backward time $t<0$, the moment is well defined for all $t \in \boldsymbol{R}$ using the relations in (28). This relation also indicates that the moments of the solution to the heat equation is completely decided by the moments of the initial time, and if two solutions share the same moments up to certain order at a certain time, then they share the same moments forever. Also note that the backward moments $\alpha_k(-t_0)$ is not a moment of a positive function even if $u_0(x)$ is positive and hence the classical theory of the moment problem is not applicable in the case.

Consider the moment problem with these backward moments:

$$\sum_{i=1}^{n} \rho_i c_i^k = \alpha_k(-t_0), \quad t_0 \geq 0,\ k = 0, 1, \cdots, 2n-1. \tag{4}$$

For the case with a positive initial value $u(x, 0) \geq 0$ and $t_0 = 0$, there exist real solutions $\rho_i, c_k \in \boldsymbol{R}$ and then the integral formula (3) is successfully replaced as $\sum_{i=1}^{n} \rho_i \phi(x - c_i, t)$ for time t large (see [15]). However, this approximation is very poor for t small since it approaches to a summation of dirac-delta distributions as $t \to 0$. Taking backward moments seems essential to obtain some regularity for the initial approximation, and hence the generalization of the moment problem is required even if the initial value is positive.

The generalization is rather simple. First introduce a positive function $\varrho_0(x) \geq 0$ which can be taken in various ways. Take its moments

$$\beta_k := \int x^k \varrho_0(x) dx, \qquad k = 0, 1, \cdots, 2n-1, \tag{5}$$

and consider a complex valued moment problem

$$\sum_{i=1}^{n} \rho_i c_i^k = m_k := \alpha_k + i\beta_k, \quad k = 0, 1, \cdots, 2n-1. \tag{6}$$

(The letter i on the right side is to denote the imaginary unit which should be distinguished from the index i from the context.) Note that the solvability of (4) is not guaranteed in general even if complex solutions are allowed. However, since the β_k's may provide extra regularity, there exists a density function $\varrho_0(x)$ such that the complex moment problem (6) is solvable (see Theorem 1).

Consider a linear combination of translations of heat kernels,

$$\Phi_n(z, t) := \sum_{i=1}^{n} \rho_i \phi(z - c_i, t), \quad t > 0,\ z \in \boldsymbol{C}, \tag{7}$$

where the heat kernel $\phi(x, t)$ is in the complex number sense, i.e.,

$$\phi(z, t) = \frac{1}{\sqrt{4\pi t}} e^{-z^2/4t}, \quad z \in \boldsymbol{C},\ t > 0. \tag{8}$$

Since the α_k's in (6) are the backward moments of the solution $u(x, t)$ at $t = -t_0$, i.e., $\alpha_k := \alpha_k(-t_0)$, the real part

$$\varphi_n(x, t) := Re(\Phi_n(x, t + t_0)) \tag{9}$$

satisfies

$$\lim_{t\to -t_0}\int x^k\varphi_n(x,t)dx = Re(\sum_{i=1}^n \rho_i c_i^k) = \alpha_k(-t_0),\quad k=0,1,\cdots,2n-1.$$

Since $\varphi_n(x,t)$ is also a solution of the heat equation, $\varphi_n(x,t)$ and $u(x,t)$ share the same moments up to order $2n-1$. This agreement of moments gives the following asymptotic convergence order (see [10, 15]):

$$\|\varphi_n(t)-u(t)\|_p = O\Big(t^{\frac{1}{2p}-\frac{2n+1}{2}}\Big)\quad \text{as}\quad t\to\infty. \tag{10}$$

Now the initial approximation $\lim_{t\to 0}\varphi_n(x,t)$ has some regularity and hence it can be a better initial approximation. In fact, if the initial value is of age $t_0>0$ (see [17]), then one may observe numerically that, for any $t\ge 0$,

$$\frac{\|u(t)-\varphi_{n+1}(t)\|_\infty}{\|u(t)-\varphi_n(t)\|_\infty}\to \frac{v}{v+2(t+t_0)}\quad \text{as}\quad n\to\infty, \tag{11}$$

where the constant $v>0$ may depend on the initial value and $t\ge 0$. This geometric convergence indicates that $\varphi_n(x,t)$ is an ideal replacement of the integral formula in (3) for all $t>0$. (Similar analysis is given in [15] for the positive solutions with $t_0=0$.)

Let a doubly indexed complex sequence α_{ij}'s satisfy $\alpha_{ij}=\overline{\alpha}_{ji}$. Then the full complex K-moment problem related to this sequence is to find a (positive) Borel measure μ that is supported on $K\subset \boldsymbol{C}$ and satisfies

$$\alpha_{ij}=\int \overline{z}^i z^j\,d\mu,\qquad i,j\ge 0. \tag{12}$$

The measure corresponding to the truncated moment problem (6) is an atomic representing measure $\mu=\sum_{i=1}^n\rho_i\delta(x-c_i)$. Depending on the choice of K, the problem is called with the names Stieltjes ($K=\boldsymbol{R}^+$), Hamburger ($K=\boldsymbol{R}$), Hausdorff ($K=[a,b]$), and Toeplitz ($K=\mathbf{T}$) (see [1,2,16,20]). If $K\subset\boldsymbol{R}$, then $\alpha_{ij}=\int x^{i+j}d\mu=\alpha_{ji}=\overline{a}_{ij}$. Therefore, the doubly indexed sequence α_{ij} is actually a singly indexed one which has real values. Hence the word 'complex' just indicates that the support K is a subset of complex numbers $\boldsymbol{C}$. (In this paper we allow the representing measure μ to have complex values and the corresponding moment sequence α_{ij}'s are truly complex valued in the sense.) This full moment problem has been extended to multidimensional spaces (see [3,18,19,21]). On the other hand, the truncated moment problem is to find a (positive) Borel measure that satisfies (12) for $0\le i,j<n$ (see [4–6,11]). If $K\subset\boldsymbol{R}$, then the problem can be written as $\alpha_k=\int x^k\,d\mu$ for $0\le k<2n$, and, if atomic representing measure is assumed, it is also written as

(1). This truncated moment problem also has been recently extended to multidimensional cases (see [7,8,12]).

There is a simpler way to control moments (see [10]). Let

$$\psi_{2n}(x,t) \equiv \sum_{k=0}^{2n-1} \frac{(-1)^k \alpha_k}{(k!)\sqrt{4\pi t}}\, \partial_x^k (e^{\frac{-x^2}{4t}}). \tag{13}$$

Then one can easily check that $\lim_{t\to 0+} \int x^k \psi_{2n}(x,t)dx = \alpha_k$ for $0 \le k < 2n$. Since ψ_{2n} is also a solution to the heat equation, it also gives the same asymptotics in (10). However, this approximate solution may diverge as $n \to \infty$ if the time $t > 0$ is not large enough (see [14]).

In this paper we have related the theory of truncated moment problem to the heat equation on the real line, and hence the Hamburger's case has been considered, i.e., $K = \boldsymbol{R}$. For boundary value problems one may consider Stieltjes or Hausdorff. To develop the approximation theory for the heat equation in a multidimensional space in the context of this paper the truncated moment theory in several variables will play the key role.

One natural question is to extend the higher asymptotic convergence order to nonlinear problems. For example, long time asymptotics of the nonlinear fast diffusion equation has been studied through spectrum analysis in [9] and the asymptotic convergence order corresponding to (10) with $n = 1$ is obtained in [13]. The same convergence order is also obtained for the Burgers equation using the Cole-Hopf transformation for $n = 1$ [14] and then for general n's taking the method in (13). The use of age of the initial profile is introduced and used in [17,23]. The technique using the backward moment in this paper seems to give a good approximation if the backward time and the age agree to each other. If one consider the initial approximations only, then the technique in this paper gives an approximation theory for general functions such as Fourier integrals or Gaussian quadrature (see Figures 1–4). These approximations also show oscillating behavior if the initial value has a discontinuity. However, the behavior such as Gibb's phenomenon appears in a different way as one may observe in Figure 4.

This paper consists as the following. In Section 2 the moment problem is generalize to a complex density function. Then, arbitrary real sequence can be embedded to a complex sequence that the corresponding complex moment problem is solvable. In Section 3 the relation for the backward moment of the heat equation is given. Approximate solutions are constructed in Section 4 using the backward moments and the extended complex moment problem. The property of approximate solution constructed without a complex part is given in Section 5. A few numerical tests of approximate solutions are given in Section 6.

2. Truncated moment problem with a complex density

In this section we extend the theory of moment problem to complex density functions. The moment problem (1) with arbitrary real α_k's will be understood as the real part of a complex moment problem. Let β_k be the k-th moment of a positive density $\varrho_0(x) \geq 0$, i.e.,

$$\beta_k = \int x^k \varrho_0(x)dx, \quad k = 0, 1, \cdots, 2n-1,$$

and m_k's be a sequence of complex numbers given by

$$m_k := \alpha_k + i\beta_k, \quad k = 0, 1, \cdots, 2n-1.$$

We will follow the routine of the classical moment problems to solve a complex valued moment problem,

$$\sum_{i=1}^{n} \rho_i c_i^k = m_k, \qquad k = 0, 1, \cdots, 2n-1, \tag{14}$$

where we are looking for complex solutions of ρ_i's and c_i's. Let $\mathbf{h}_k \in \boldsymbol{C}^{n\times 1}$ be a column vector and $H \in \boldsymbol{C}^{n\times n}$ be the Hankel matrix given by

$$\begin{array}{ll} \mathbf{h}_k := (m_k, m_{k+1}, \cdots, m_{k+n-1})^t, & k = 0, 1, \cdots, n, \\ H := (m_{i+j}), & i, j = 0, 1, \cdots, n-1. \end{array} \tag{15}$$

(Here, $\boldsymbol{C}^{m\times n}$ stands for the collection of $m \times n$ complex matrices.) Note that these Hankel matrices are symmetric and the j-th column is $\mathbf{h}_{j-1}$. Similarly, we construct the Hankel matrices and column vectors corresponding to the real sequences α_k's and β_k's:

$$\begin{array}{ll} \mathbf{a}_k := (\alpha_k, \alpha_{k+1}, \cdots, \alpha_{k+n-1})^t, & k = 0, 1, \cdots, n, \\ \mathbf{b}_k := (\beta_k, \beta_{k+1}, \cdots, \beta_{k+n-1})^t, & k = 0, 1, \cdots, n, \\ A := (\alpha_{i+j}), & i, j = 0, 1, \cdots, n-1, \\ B := (\beta_{i+j}), & i, j = 0, 1, \cdots, n-1. \end{array} \tag{16}$$

The Hankel matrices and the moment vectors satisfy

$$H = A + iB, \quad \mathbf{h}_k = \mathbf{a}_k + i\mathbf{b}_k, \quad k = 0, 1, \cdots, n.$$

Let $0 \neq \mathbf{y} \in \boldsymbol{R}^{n\times 1}$. Then,

$$\begin{aligned} \mathbf{y}^t B \mathbf{y} = \sum_{i,j=0}^{n-1} y_i y_j \beta_{i+j} &= \int \Big(\sum_{i,j=0}^{n-1} y_i x^i y_j x^j \Big) \varrho_0(x)dx \\ &= \int \Big(\sum_{k=0}^{n-1} y_k x^k \Big)^2 \varrho_0(x)dx > 0. \end{aligned}$$

Hence, the symmetric matrix B is positive definite.

Lemma 1. *Let A and B be $n \times n$ real symmetric matrices. If B is positive definite, then*
(i) The matrix $H := A + iB$ is non-singular.
(ii) For $\mathbf{z} \in \boldsymbol{C}^n$,

$$\overline{\mathbf{z}}^t H\mathbf{z} = 0 \iff \mathbf{z} = 0.$$

Proof. Let $\mathbf{z} := \mathbf{x} + i\mathbf{y}$ with $\mathbf{x}, \mathbf{y} \in \boldsymbol{R}^{n\times 1}$ satisfy $H\mathbf{z} = 0$. Then, the linear system $H\mathbf{z} = 0$ can be written as

$$\begin{pmatrix} H_{2n} \end{pmatrix} \begin{pmatrix} \mathbf{y} \\ \mathbf{x} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \quad \begin{pmatrix} H_{2n} \end{pmatrix} := \begin{pmatrix} B & A \\ A & -B \end{pmatrix}. \tag{17}$$

Hence the singularity of the complex $n \times n$ matrix H is same as the one of the $2n \times 2n$ matrix H_{2n}. Since the matrix B is invertible, a block elimination gives

$$\begin{pmatrix} I & 0 \\ -AB^{-1} & I \end{pmatrix} \begin{pmatrix} B & A \\ A & -B \end{pmatrix} = \begin{pmatrix} B & A \\ 0 & -(B + AB^{-1}A) \end{pmatrix}.$$

Since B is invertible, there exists $\tilde{\mathbf{x}} \in \boldsymbol{R}^{n\times 1}$ such that $B\tilde{\mathbf{x}} = A\mathbf{x}$. Therefore,

$$\mathbf{x}^t AB^{-1}A\mathbf{x} = (B\tilde{\mathbf{x}})^t B^{-1} B\tilde{\mathbf{x}} = \tilde{\mathbf{x}}^t B\tilde{\mathbf{x}} \geq 0,$$

and hence $AB^{-1}A$ is at least semi-positive definite. Finally we have that the Schur martix $-(B + AB^{-1}A)$ is negative definite and

$$\det(H_{2n}) = -\det(B)\det(B + AB^{-1}A) < 0,$$

which completes the proof of the first part (i).

Let $\mathbf{z} = \mathbf{x} + i\mathbf{y}$ satisfy $\overline{\mathbf{z}}^t H\mathbf{z} = 0$, i.e.,

$$\overline{\mathbf{z}}^t H\mathbf{z} = (\mathbf{x}^t A\mathbf{x} + \mathbf{y}^t A\mathbf{y}) + i(\mathbf{x}^t B\mathbf{x} + \mathbf{y}^t B\mathbf{y}) = 0.$$

Since B is positive definite and $\mathbf{x}^t B\mathbf{x} + \mathbf{y}^t B\mathbf{y} = 0$, we have $\mathbf{x} = 0 = \mathbf{y}$ and hence $\mathbf{z} = 0$. $\square$

Since H is invertible, there exists a solution $\Psi = (\psi_0, \cdots, \psi_{n-1})^t$ that satisfies

$$H\Psi = \mathbf{h}_n. \tag{18}$$

This can be written as $\sum_{j=0}^{n-1} \psi_j \mathbf{h}_j = \mathbf{h}_n$ or

$$m_{n+k} - \sum_{j=0}^{n-1} \psi_j m_{j+k} = 0, \quad k = 0, 1, \cdots, n-1. \tag{19}$$

Introduce an auxiliary polynomial,

$$g_n(z) := z^n - \sum_{j=0}^{n-1} \psi_j z^j, \quad z \in \boldsymbol{C}. \tag{20}$$

Due to the fundamental theorem of algebra, there exist n complex zeros of the polynomial $g_n(z)$ including multiplicities.

The next step is to investigate the multiplicity of zeros of the auxiliary polynomial $g_n(z)$. To do that we consider a linear functional $S(f)$ defined for a polynomial. For a given polynomial $f(z) = \sum_{i=0}^{l} f_i z^i$, $S(f)$ is defined by

$$S(f) := f_0 m_0 + \cdots + f_l m_l = \sum_{i=0}^{l} f_i m_i = \sum_{i=0}^{l} f_i(\alpha_i + i\beta_i). \tag{21}$$

One may easily see that this is a linear functional and gives the expectation of the polynomial restricted on the real line if the sequence m_i's are moments of a probability function. For example, if $m_k = \int x^k p(x)dx$ for all k, then

$$S(f) = \sum_{i=0}^{l} f_i m_i = \sum_{i=0}^{l} f_i \int x^i p(x) = \int f(x)p(x)dx. \tag{22}$$

Remark 1. Since we are interested in the application to the solutions of the heat equation in the real line, the moments m_k's and the functional $S(f)$ are defined as the line integral along the real axis. In general one may consider a contour integral and define

$$S(f) := \oint_C f(z)p(z)dz = \int_0^1 f(z(t))p(z(t))z'(t)dt,$$

where $z = z(t)$ is a parametrization of a closed curve C. For the case with the unit circle is called ... (see [**?**]).

We set the conjugate of the polynomial $f(z) = \sum_{i=0}^{l} f_i z^i$ as

$$\overline{f}(z) := \sum_{i=0}^{l} \overline{f}_i z^i.$$

In the followings we consider basic properties related to this functional and the zeros of the auxiliary polynomial $g_n(z)$.

Lemma 2. *Let the imaginary part of m_k's be given by a positive density as in (6) and the linear functional $S(f)$ is given by (21). Then,*
(i) If $f \neq 0$, then $S(\overline{f}f) \neq 0$.
(ii) If $f(z) = (z - c_1)\cdots(z - c_k)$, then $\overline{f}(z) = (z - \overline{c}_1)\cdots(z - \overline{c}_k)$.

(iii) The auxiliary polynomial $g_n(z)$ given by (20) satisfies

$$S(g_n(z)z^k) = 0, \qquad k = 0, 1, \cdots, n-1. \tag{23}$$

Proof. (i) Let $0 \neq f(z) = \sum_{i=0}^{l} f_i z^i$. Then, $\overline{f}(z)f(z) = \sum_{i,j=0}^{k} \overline{f}_i f_j z^{i+j}$. Therefore, by Lemma 1$(ii)$,

$$S(\overline{f}f) = \sum_{i,j=0}^{k} \overline{f}_i f_j m_{i+j} = \overline{\mathbf{f}}^t H \mathbf{f} \neq 0,$$

where $\mathbf{f} = (f_0, f_1, \cdots, f_l)^t$.

(ii) Let $f(z) = (z-c_1)\cdots(z-c_k) = \sum_{i=0}^{k} f_i z^i$. Then, the coefficients f_i's are given by

$$f_i = \sum_{I \in A_i} \Big(\prod_{j \in I} c_j \Big),$$

where A_i is the collection of all index sets consists of $k-i$ indices. Hence,

$$\overline{f}_i = \overline{\sum_{I \in A_i} \Big(\prod_{j \in I} c_j \Big)} = \sum_{I \in A_i} \Big(\prod_{j \in I} \bar{c}_j \Big).$$

In other words $\overline{f}(z) = (z-\bar{c}_1)\cdots(z-\bar{c}_k)$. The last claim (iii) is obtained by comparing (19) and (20), i.e.,

$$S(g_n(z)z^k) = m_{n+k} - \sum_{j=0}^{n-1} \psi_j m_{j+k} = 0, \quad k = 0, 1, \cdots, n-1.$$

□

Lemma 3. *Let the imaginary part of m_k's be given by a positive density as in (6) and the linear functional $S(f)$ is given by (21). Then,*
(i) If $c \in \boldsymbol{C} \setminus \boldsymbol{R}$ is a zero of $g_n(z)$, then its conjugate $\bar{c}$ is not.
(ii) There is no real zero of $g_n(z)$ with multiplicity two or higher.
(iii) If $\alpha_k = 0$ for all k's and $\varrho_0(x) \geq 0$ is non-trivial, then $g_n(z)$ has n-distinct complex zeros.

Proof. (i) Suppose that c and its conjugate $\bar{c}$ are zeros of the polynomial $g_n(z)$. Then one may write

$$g_n(z) = (z-c)(z-\bar{c})(z-c_3)\cdots(z-c_n).$$

Let $h(z) = (z-c)(z-c_3)\cdots(z-c_n)$. Then,

$$g_n(z)(z-\bar{c}_3)\cdots(z-\bar{c}_n) = \bar{h}(z)h(z).$$

The linearity of the operator S and Lemma 2(iii) imply that

$$S(g_n(z)(z-\bar{c}_3)\cdots(z-\bar{c}_n)) = 0.$$

However, Lemma 1(ii) implies that $S(\bar{h}h) \neq 0$, which contradicts. Therefore, if a $c \in \boldsymbol{C}$ is a zero of $g_n(z)$, then its conjugate $\bar{c}$ is not.

(ii) Suppose that $g_n(z)$ has a real zero of multiplicity of two or higher, say $a \in \boldsymbol{R}$. Then we may write

$$g_n(z) = (z-a)^2(z-c_3)(z-c_4)\cdots(z-c_n).$$

Let $h(z) = (z-a)(z-c_3)\cdots(z-c_n)$. Then, since $\bar{a} = a$,

$$g_n(z)(z-\bar{c}_3)\cdots(z-\bar{c}_n) = \bar{h}(z)h(z).$$

The arguments in the previous step derive the same contradiction. Therefore, $g_n(z)$ has no real zero of multiplicity two or higher.

(iii) Suppose that $c = a + ib$ is a complex zero of $g_n(z)$ with multiplicity two or higher. First, $b \neq 0$ from (ii). Then we may write

$$g_n(z) = ((z-a)-ib)^2 h(z), \qquad h(z) = (z-c_3)\cdots(z-c_n).$$

Since $(z-a)\bar{h}(z)$ is a polynomial of degree $n-1$, the linearity of S and Lemma 2(iii) imply that $S(g_n(z)(z-a)\bar{h}(z)) = 0$. Since $a_k = 0$ for all k, $m_k = \beta_k$ and hence

$$S(g_n(z)(z-a)\bar{h}(z)) = i\int[(x-a)^3 - b^2(x-a) - 2ib(x-a)^2]\bar{h}(x)h(x)\varrho_0(x)dx.$$

The real part gives

$$\int 2b(x-a)^2\bar{h}(x)h(x)\varrho_0(x)dx = 0.$$

Since the integrand is non-negative, it contradicts to the assumption that $\varrho_0(x) \geq 0$ is non-trivial. Hence, there is no zero of multiplicity two or higher. □

Remark 2. For the real moment problem case the polynomial corresponding to $g_n(z)$ has real zeros only, and all of them are of multiplicity one. Lemma 3(ii) says that the real zeros of the complex polynomial $g_n(z)$ are also of multiplicity one for any choice for the density function $\varrho_0(x) \geq 0$ of the imaginary part. It is also shown that the complex zeros are also of multiplicity one assuming trivial real parts. We could not obtain such a result under a general choice of α_k's and $\varrho_0(x) \geq 0$ and left it as a conjecture. However, we can easily show the existence of such a density function $\varrho_0(x) \geq 0$ for given α_k's.

Theorem 1. *Let a sequence $\alpha_k \in \boldsymbol{R}$, $0 \leq k < 2n$, be given. Then, there exists a positive density function $\varrho_0(x) \geq 0$ such that the sequence of complex moments,*

$$m_k := \alpha_k + i\beta_k \quad \textit{with} \quad \beta_k := \int x^k \varrho_0(x)dx, \quad 0 \leq k < 2n,$$

has the following properties.

(i) The polynomial $g_n(z) := z^n - \sum_{i=0}^{n-1} \psi_i z^i$ *has n-distinct zeros, where* $\Psi := (\psi_0, \cdots, \psi_{n-1})^t$ *solves (18).*
(ii) The truncated complex moment problem,

$$\sum_{i=1}^{n} \rho_i c_i^k = m_k (:= \alpha_k + i\beta_k), \qquad k = 0, 1, \cdots, 2n-1, \tag{24}$$

has a unique solution $\rho_i, c_i \in \boldsymbol{C}$*.*

Proof. (i) Let $f(x) \geq 0$ be a non-trivial positive function and

$$\gamma_k(\tau; , f) = \tau\alpha_k + f_k, \qquad f_k := \int x^k f(x)dx.$$

For a given $\tau \geq 0$, let $g_n(z; f, \tau)$ be the auxiliary polynomial given by the moments $\gamma_k(\tau, f)$. (Hence, $g_n(z)$ in the theorem can be written as $g_n(z; \varrho_0, 1)$. The existence of the polynomial is clear since the Hankel matrix H is nonsingular.) We already know that $g_n(z; f, 0)$ has n-distinct zeros, Lemma 3(iii), and hence there exists $\tau_0 > 0$ such that $g_n(z; f, \tau_0)$ also has n-distinct zeros. Set $\varrho_0(x) := f(x)/\tau_0$. Then, since $\beta_k := \int x^k \varrho_0(x)dx = f_k/\tau_0$,

$$\gamma_k(f, \tau_0) = \tau_0\alpha_k + f_k = \tau_0(\alpha_k + \beta_k) =: \tau_0 m_k.$$

Therefore, the corresponding linear systems (18) to the two sequences $\gamma_k(f, \tau_0)$ and m_k are identical and hence $g_n(z) = g_n(z; f, \tau_0)$, which completes the proof of part (i).

(ii) Now we show the solvability of the complex moment problem (24). (The proof is essentially same as the real moment problem case.) Let c_i's be the n distinct zeros of the polynomial $g_n(z)$ for $i = 1, \cdots, n$. Since c_i's are distinct, there exists a unique solution that solves the first n equations in (24), i.e., for $0 \leq k < n$. Now we complete the proof using inductive arguments. Let $0 \leq l \leq n-1$. We will show that the equation in (24) holds for $k = n_0 + l$ under the assumption that equations hold for all $0 \leq k < n_0 + l$. First observe that, since c_i's are zeros of $z^l g_n(z), l \geq 0$,

$$c_i^{n+l} = \sum_{j=0}^{n-1} \psi_j c_i^{j+l} \qquad \text{for any} \quad 1 \leq i \leq n_0,\ k \geq 0.$$

Using the relations (24) and (19) for $k < n + l$, we obtain

$$m_{n+l} = \sum_{j=0}^{n-1} \psi_j m_{j+l} = \sum_{j=0}^{n-1} \psi_j \sum_{i=1}^{n} \rho_i c_i^{j+l} = \sum_{i=1}^{n} \rho_i \sum_{j=0}^{n-1} \psi_j c_i^{j+l} = \sum_{i=1}^{n} \rho_i c_i^{n+l}.$$

Hence, (24) holds for $k = n + l$ and hence for all $k = 0, 1, \cdots, 2n-1$ by induction. $\square$

Remark 3. In general the moment problem $\sum_{i=1}^{n} \rho_i c_i^k = \alpha_k$, $0 \le k < 2n$, does not have a solution. However, Theorem 1 implies that there always exist ρ_i's and c_i's such that

$$Re\Big(\sum_{i=1}^{n} \rho_i c_i^k\Big) = \alpha_k, \qquad k = 0, 1, \cdots, 2n-1. \tag{25}$$

There are various ways to construct such ρ_i's and c_i's. If a positive density $\varrho_0(x) \ge 0$ is given, one may construct one set of ρ_i's and c_i's. However, we do not have a criterion to choose the best one.

3. Moments of the backward heat equation

Let $w(z,t)$ be the solution to the complex heat equation with a complex initial value, i.e.,

$$w_t = w_{zz}, \quad w(z,0) = w_0(z), \qquad z, w \in \boldsymbol{C}. \tag{26}$$

It is assumed that the initial value $w_0(z)$ decays fast enough as $|z| \to \infty$ to get the k-th order moment $\gamma_k(t)$ be well defined,

$$\gamma_k(t) = \int_{-\infty}^{\infty} x^k w(x,t)dx, \quad k = 0, 1, \cdots, 2n-1 \tag{27}$$

at least for the initial time $t = 0$. One can easily show how these moments evolve as t varies.

Lemma 4. *Suppose that the initial value $w_0(x)$ has finite moments up to $2n$-th order, i.e., $x^{2n}w_0(x) \in L^1(\boldsymbol{R})$. Then the moments of the solution $w(x,t)$ at time $t \ge 0$ are given by*

$$\begin{aligned} \gamma_{2k}(t) &= \textstyle\sum_{l=0}^{k} \frac{(2k)!}{(k-l)!(2l)!} t^{k-l} \gamma_{2l}(0), \\ \gamma_{2k+1}(t) &= \textstyle\sum_{l=0}^{k} \frac{(2k+1)!}{(k-l)!(2l+1)!} t^{k-l} \gamma_{2l+1}(0). \end{aligned} \tag{28}$$

Furthermore, the linear combinations in (28) are well defined for all $t \in \boldsymbol{R}$ and identical to the moments of the solution to the backward heat equation if it is solvable up to the given time.

Proof. Integrating by parts gives

$$\begin{aligned} \gamma_0'(t) &= \int w_t dx = \int w_{xx} dx = [w_x]_{-\infty}^{\infty} = 0, \\ \gamma_1'(t) &= \int x w_t dx = \int x w_{xx} dx = [x w_x - w]_{-\infty}^{\infty} = 0. \end{aligned}$$

Hence, $\gamma_0(t)=\gamma_0(0)$ and $\gamma_1(t)=\gamma_1(0)$ are constants which gives (28) for $k=0$ and $k=1$. For $k\ge 2$,

$$\begin{aligned}\gamma_k'(t) &= \int x^k w_t dx = \int x^k w_{xx} dx\\ &= [x^k w_x - kx^{k-1}w]_{-\infty}^{\infty} + \int k(k-1)x^{k-2} w dx\\ &= k(k-1)\gamma_{k-2}(t).\end{aligned}$$

Hence, in summary, we have

$$\frac{d}{dt}\gamma_k(t) = \begin{cases} 0\,, & k=0 \text{ or } 1,\\ k(k-1)\gamma_{k-2}(t), & k\ge 2.\end{cases}$$

This relation shows that the even numbered moments and the odd numbered ones evolve separately and can be obtained inductively by integrating lower order moments from $\gamma_0(t)$ or $\gamma_1(t)$ which are constants. The formulas in (28) can be easily verified in that manner.

Consider a column vector $\mathbf{m}_{2n}(t)=(\gamma_0(t),\cdots,\gamma_{2n-1}(t))^t$ and the $2n\times 2n$ matrix $A(t)$ that consists of the coefficients in (28). Then,

$$\mathbf{m}_{2n}(t) = A(t)\mathbf{m}_{2n}(0).$$

One may easily check that the matrix multiplication $A(t)A(-t)$ is the identity matrix for all $t>0$. Hence $A(t)$ is non-singular and the last sentence of the lemma is clear. □

An initial heat distribution w_0 is called of age $t_0\ge 0$ if there exists a function $\tilde{w}_0(x)$ such that the solution $\tilde{w}(x,t)$ to the heat equation with $\tilde{w}_0$ as its initial value satisfies $\tilde{w}(x,t_0)=w_0(x)$ for all $x\in\boldsymbol{R}$ and the $t_0\ge 0$ is the maximum to have such a function $\tilde{w}_0$. One may find an estimate of such an age for a positive case from [17]. However, this lemma indicates that moments of the solution to the backward heat equation can be easily computed even if the backward problem itself is not solvable. This is not strange at all. Since for any given $t_0>0$ there may exist $W_0(x)$ such that it has an age of older than t_0 and shares the same moments up to order $2n-1$ with $w_0(x)$. Then the backward moments are the ones for the initial value $W_0(x)$.

4. Truncated moment problem with moments from the past

Let $u(x,t)$ be the solution of the heat equation with a real initial value $u_0(x)$ where $x^{2n}u_0(x)$ is integrable. Let $\alpha_k(t)$ be the k-th order moments at time $t\in\boldsymbol{R}$, i.e.,

$$\alpha_k(t) := \int x^k u(x,t)dx, \qquad k=0,1,\cdots,2n-1. \tag{29}$$

Then, for $t_0 > 0$, the backward moment $\alpha_k(-t_0)$ is well defined by (28). Let $\varrho_0(x) \geq 0$ be the density function in Theorem 1 corresponding to the sequence $\alpha_k := \alpha_k(-t_0)$ and $\varrho(x,t)$ be the solution of the heat equation

$$\varrho_t = \varrho_{xx}, \quad \varrho(x,-t_0) = \varrho_0(x).$$

Then, Theorem 1 says that, for

$$\beta_k(t) := \int x^k \varrho(x,t)dx, \qquad k = 0, 1, \cdots, 2n-1, \tag{30}$$

there exist $\rho_i, c_i \in \boldsymbol{C}$ that satisfy

$$\sum_{i=1}^{n} \rho_i c_i^k = m_k := \alpha_k(-t_0) + \beta_k(-t_0). \tag{31}$$

Now we employ these ρ_i's and c_i's to construct an approximation

$$\Phi_n(z,t) \equiv \sum_{i=1}^{n} \frac{\rho_i}{\sqrt{4\pi t}}\, e^{-(z-c_i)^2/4t}. \tag{32}$$

It is clear that this linear combination of complex heat kernels is also a solution to the heat equations. Let

$$w(x,t) = u(x,t) + i\varrho(x,t).$$

Then, due to the linearity of the heat equation, the complex valued function $w(x,t)$ is a solution to the heat equation

$$w_t = w_{xx}, \quad w(x,0) = u_0(x) + i\varrho(x,0), \quad t > 0,\ x \in \boldsymbol{R}. \tag{33}$$

Since $\Phi_n(z,t) \to \sum_{i=1}^{n} \rho_i \delta(z - c_i)$ as $t \to 0$, the initial moments of $\Phi_n(z,t)$, $0 \leq k < 2n$, are given by

$$\lim_{t\to 0} \int x^k \Phi_n(x,t)dx = \sum_{i=1}^{n} \rho_i c_i^k = \alpha_k(-t_0) + i\beta(-t_0). \tag{34}$$

Therefore, from the relations (28), we may conclude that $\Phi_n(x, t+t_0)$ and $w(x,t)$ shares the same moments up to order $2n-1$. If the real parts are compared, then

$$\int x^k u(x,t)dx = \int x^k Re(w(x,t))dx = \int x^k Re(\Phi_n(x, t+t_0))dx,$$

and hence the solution $u(x,t)$ and the real part of the approximation $Re(\Phi_n(x,t+t_0))$ share the same moments up to order $2n-1$. Let

$$\varphi_n(x,t) := Re(\Phi_n(x, t+t_0)).$$

Then $\varphi_n(x,t)$ is the approximation of the solution $u(x,t)$ which is our candidate to replace the integral formula of the solution .

We summarize the results in the following theorem.

Theorem 2. *Let $u(x,t)$ be the solution to the heat equation with an initial value $u_0(x)$ such that $x^{2n}u_0(x)$ is integrable. Then, for any given $t_0>0$, there exist $\rho_i, c_i \in \boldsymbol{C}$ such that*

$$\int x^k \varphi_n(x,t)dx = \int x^k u(x,t)dx, \quad k=0,1,\cdots,2n-1, \tag{35}$$

where

$$\varphi_n(x,t) := Re\Big(\sum_{i=1}^n \frac{\rho_i}{\sqrt{4\pi(t+t_0)}}\, e^{-(x-c_i)^2/4(t+t_0)}\Big). \tag{36}$$

Note that $u(x,t)$ and $\varphi_n(x,t)$ are getting smeared under the same mechanism as t increases and share the same moments up to order $2n-1$ forever. Hence, it is natural to expect that $\varphi_n(x,t)$ approaches to $u(x,t)$ fast as $t\to\infty$. In fact higher order convergence orders have been obtained in [10, 15] using the agreement of moments, which is the same order given in the following theorem. The proof is basically same as the ones in [15] and hence skipped here.

Theorem 3. *Let $u(x,t)$ and $\varphi_n(x,t)$ be the ones in Theorem 2 under the same conditions. Then, for $1\le p\le\infty$,*

$$\lim_{t\to\infty} t^{\frac{2n+1}{2}-\frac{1}{2p}}\|\varphi_n(t)-u(t)\|_p = \frac{\|\partial_x^m(e^{\frac{-x^2}{4}})\|_p}{\sqrt{4\pi}}\Big|\int E_{2n}(x)dx\Big| < \infty, \tag{37}$$

where

$$E_0(x) := \varphi_n(x,0)-u(x,0)$$

and

$$E_k(x) := \int_{-\infty}^x E_{k-1}(y)dy,\ 0<k\le 2n. \tag{38}$$

Remark 4. This simple theorem gives a surprising conclusion. Even if the $n\times n$ Hankel matrix of a real valued solution $u(x,t)$ is singular, one may construct a complex valued approximation $\Phi_n(z,t)$ defined on the complex plane by choosing an imaginary initial value, say $\varrho_0(x) := \phi(x,\epsilon)$ for example. There are various kinds of choices for the imaginary part and a different kind of imaginary part gives a different approximation. However, all of them shares the same real part of their moments and hence they show good behavior for $t>0$ large and $n>0$ large. It is natural to ask a criterion to choose the best imaginary part $\varrho_0(x)\ge 0$ in a unique way. However, we do not have one.

Remark 5. The approximation $\varphi_n(x,t)$ has some regularity even for the initial time $t=0$ thanks to the $t_0>0$ in (36). This improves the initial approximation, in particular, if the initial value u_0 is smooth. It is natural to ask what is the optimal t_0 to obtain the best approximation result. Unfortunately, we do not have an answer.

5. Real initial value case

In this section we consider the complex moment problem with zero imaginary part $\varrho_0(x) = 0$. In other words we consider complex solutions $\rho_i, c_i \in \boldsymbol{C}$ that solve

$$\sum_{i=1}^{n} \rho_i c_i^k = \alpha_k \in \boldsymbol{R}, \quad k = 0, 1, \cdots, 2n-1. \tag{39}$$

It is well-known that, if α_k's are moments of a positive function, this problem has real solutions. Here we are interested in the case that α_k's are not necessarily moments of a positive function. This moment problem is not solvable in general even if complex solutions are considered. In particular the Hankel A given in (16) can be singular. In this section we consider the property of solutions of the moment problem and the approximation solution

$$\Phi_n(z,t) \equiv \sum_{i=1}^{n} \frac{\rho_i}{\sqrt{4\pi t}} e^{-(z-c_i)^2/4t}$$

for the case that (39) is solvable.

Theorem 4. *Let α_k's be real numbers. Suppose that the Hankel matrix $A = (\alpha_{i+j})$ is non-singular and the auxiliary polynomial $g_n(z)$ has n distinct zeros. If c_i is a complex zero of the polynomial $g_n(z)$, then its conjugate $\bar{c}_i$ is also a zero. Furthermore, if $c_j = \bar{c}_i$, then $\rho_j = \bar{\rho}_i$. The restriction of $\Phi_n(z,t)$ to the real line is real valued.*

Proof. Since the α_k's are real, the Hankel matrix A and the vector $\mathbf{a}_n$ in (16) are real valued. Hence the solution Ψ to the linear problem $A\Psi = \mathbf{a}_n$ consists of real numbers and hence the polynomial $g_n(z) = z^n - \sum_{k=0}^{n-1} \psi_k z^k$ is of real coefficients. Hence if $g_n(z)$ has a complex zero, its conjugate is also a zero.

Now we show that the ρ_i's that solve the first n equations in (39) satisfy $\rho_j = \bar{\rho}_i$ if $c_j = \bar{c}_i$. After a reordering we may assume that $c_{2j-1} = \overline{c_{2j}}$ for $j = 1, \cdots, l$ and c_i's are real numbers for $j > 2l$. Let

$$a_{k,2j-1} := c_{2j-1}^{k-1} + c_{2j}^{k-1}, \quad a_{k,2j} := i(c_{2j-1}^{k-1} - c_{2j}^{k-1}).$$

Then, since $c_{2j-1} = \overline{c_{2j}}$, these $a_{k,i}$'s are real numbers for $0 < i \le 2l$. We should show that the solution ρ_i's are given in the form of $\rho_{2j-1} = x_{2j-1} + ix_{2j}$ and $\rho_{2j} = x_{2j-1} - ix_{2j}$ for $j = 1, \cdots, l$. One may easily check that the existence of such x_i's for $1 \le i \le 2l$ is equivalent to the existence of real solutions to the following linear system with real coefficients:

$$\begin{pmatrix} a_{1,1} & \cdots & a_{1,2l} & c_{2l+1}^{0} & \cdots & c_n^{0} \\ \vdots & \cdots & \vdots & \vdots & \cdots & \vdots \\ a_{2l,1} & \cdots & a_{2l,2l} & c_{2l+1}^{2l-1} & \cdots & c_n^{2l-1} \\ a_{2l+1,1} & \cdots & a_{2l+1,2l} & c_{2l+1}^{2l} & \cdots & c_n^{2l} \\ \vdots & \cdots & \vdots & \vdots & \cdots & \vdots \\ a_{n,1} & \cdots & a_{n,2l} & c_{2l+1}^{n-1} & \cdots & c_n^{n-1} \end{pmatrix} \begin{pmatrix} x_1 \\ \vdots \\ x_{2l} \\ \rho_{2l+1} \\ \vdots \\ \rho_n \end{pmatrix} = \begin{pmatrix} \alpha_0 \\ \vdots \\ \alpha_{2l-1} \\ \alpha_{2l} \\ \vdots \\ \alpha_{n-1} \end{pmatrix}. \quad (40)$$

One may easily check that the real matrix is obtained from the $n \times n$ Vandermonde matrix that gives the first n-equations in (39) by simply adding two columns or subtracting one from another. (Remember that the ij-component of the Vandermonde matrix is c_j^{i-1}.) One may also easily show that the $n \times n$ matrix in (40) is invertible since the Vandermonde is invertible. In other words there exist ρ_i's and c_i's satisfying the claims of the theorem. Since the solution to the moment problem is unique, these are the ones.

Let x be a real number. Then

$$\frac{\overline{\rho}}{\sqrt{4\pi t}}\, e^{-(x-\overline{c})^2/4t} = \overline{\frac{\rho}{\sqrt{4\pi t}}\, e^{-(x-c)^2/4t}}$$

Therefore,

$$\frac{\rho_{2j-1}}{\sqrt{4\pi t}}\, e^{-(x-c_{2j-1})^2/4t} = \overline{\frac{\rho_{2j}}{\sqrt{4\pi t}}\, e^{-(x-c_{2j})^2/4t}}, \quad 1 \le j \le l.$$

It is now clear that the restriction of $\Phi_n(z,t)$ to the real line is real valued. □

Even if the moment problem (39) is not solvable in general, such a case is very rare in the sense that it is of measure zero case. Hence the point is that complex solutions should be included. It seems that extension of the heat equation to the complex case will give many benefits. Furthermore, even if ρ_i's and c_i' are complex numbers, the restriction of $\Phi_n(z,t)$ to the real numbers has real values.

6. Structure of the approximation

In this section we numerically investigate the property of the approximation

$$\varphi_n(x,t) := Re\Big(\sum_{i=1}^{n} \frac{\rho_i}{\sqrt{4\pi(t+t_0)}}\, e^{-(z-c_i)^2/4(t+t_0)}\Big),$$

which was constructed in the previous sections. This approximation is decided by the choice of the backward time t_0 and the imaginary part $\varrho_0(x)$. We do not have a criterion to choose the t_0 and ϱ_0. In this section we just observe how these choices may make differences.

6.1. Approximation using a single heat kernel

Examples that clearly show the benefit of using the complex moment problem over the real one are the single heat kernel cases, i.e., $n = 1$. Fundamental solutions are frequently employed as canonical solutions of various problems. In many cases fundamental solutions are given explicitly and play key roles in the analysis of general solutions. For the heat equation case it is given by the Gaussian which is also called the heat kernel. This real valued heat kernel is a signed function and does not show a sign-changing property. In the following examples we will see how a single heat kernel in the complex plane can show the behavior of sign-changing solutions on the real line.

For the first example, consider an initial value

$$u_0(x) := \frac{1}{\sqrt{4\pi}} e^{\frac{-(x+1)^2}{4}} - \frac{1}{\sqrt{8\pi}} e^{\frac{-x^2}{8}}. \tag{41}$$

Then the first two moments of the solution $u(x,t)$ are given by

$$\alpha_0(t) = 0, \quad \alpha_1(t) = 1.$$

Since they are constants, the backward moments are also given by $\alpha_0(-t_0) = 0$ and $\alpha_1(-t_0) = 1$ for any backward time $t_0 > 0$. For the case $n = 1$, the complex function $\Phi_1(z,t) = \frac{\rho_1}{\sqrt{4\pi t}} e^{\frac{-(z-c_1)^2}{4t}}$ should be obtained by solving the following two moment equations

$$\rho_1 = 0, \qquad c_1\,\rho_1 = 1.$$

However, in this case, the corresponding 1×1 Hankel matrix A is the zero matrix which is singular. It is clear that this moment problem is not solvable even if the complex solutions are allowed. Therefore, one should introduce an imaginary part. Let $w(x,t)$ be a complex valued solution to the heat equation with an initial value

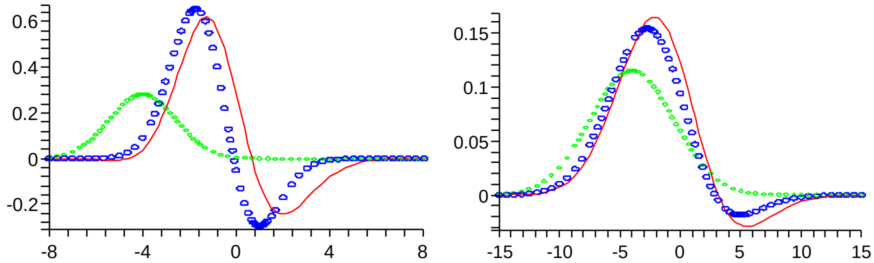
$$w_0(x) := u_0(x) + i\varrho_0(x), \quad \varrho_0(x) := \phi(x + 0.5, 1),$$

where $\phi(x,t)$ is the heat kernel. Then the real part of the complex solution $w(x,t)$ is just $u(x,t)$ for any choice of the imaginary part $\varrho_0(x)$. However, the real part of its approximation $\Phi_1(x,t)$ depends on the choice of $\varrho_0(x)$. Under the above choice of $\varrho_0(x)$, the first two moments are given by $\alpha_0(t) = i$ and $\alpha_1(t) = 1 - 0.5i$. Then the corresponding moment equations are

$$\rho_1 = i, \qquad c_1\,\rho_1 = 1 - 0.5i.$$

The solution of the moment problem is

$$\rho_1 = i, \qquad c_1 = -0.5 - i.$$



(a) Initial approximation (b) Approximations at time $t = 5$

Fig. 1. The exact solution is given in a red line. Single heat kernel using a real Gaussian is given in black lines. However, the complex Gaussian with an imaginary part, blue dots, gives sign-changing behavior.

Let $\varphi_1(x,t)$ be the restriction of the real part of the approximation $\Phi_1(z,t)$ to the real line, i.e., $\varphi_1(x,t) := Re(\frac{\rho_1}{\sqrt{4\pi(t+1)}} e^{-(x-c_1)^2/4(t+1)})$. Note that we are using the backward time $t_0 = 1$ here. Then the optimal convergence order in [15] is obtained as

$$\lim_{t\to\infty} t^{(\frac{3}{2}-\frac{1}{2p})} \|u(t) - \varphi_1(t)\|_p = \frac{\|\partial_\xi^2 (e^{-\frac{1}{4}\xi^2})\|_p}{\sqrt{4\pi}} \Big| \int_{-\infty}^{\infty} E_2(x)dx \Big|,$$

where $1 \le p \le \infty$ and

$$E_2(x) = \int_{-\infty}^{x} \int_{-\infty}^{y} [\varphi_1(s,0) - u_0(s)] ds dy.$$

Hence, we have obtained the optimal convergence order using the generalized moment problem even if the corresponding Hankel matrix for the initial value $u_0(x)$ is singular.

If $\alpha_0 \neq 0$, then the approximation of the optimal order can be obtained without using an imaginary part. For the second example, consider such a case with an initial value

$$u_0(x) := \frac{4}{\sqrt{4\pi}} e^{\frac{-(x+1)^2}{4}} - \frac{3}{\sqrt{8\pi}} e^{\frac{-x^2}{8}}. \tag{42}$$

This initial value is given in Figure 1(a) with a (red) line. Then, the zero-th moment is $\alpha_0 = 1$ and hence the Hankel matrix A is non-singular. The approximation without the imaginary part has been computed using a backward time $t_0 = 1$ which is given in Figure 1(a) in (green) dots. In this case the approximation is a positive function. On the other hand an approximation using the following imaginary part,

$$\varrho_0(x) = 4\phi(x + 0.5, 1)\Big(= \frac{4}{\sqrt{4\pi}} e^{\frac{-(x+0.5)^2}{4}}\Big),$$

is given in (blue) circles. Notice that, since the backward moments were used, the initial approximations are not spiky and the initial difference is not so big even if only one heat kernel is used. Furthermore, the case with complex density function, the behavior of sign-change is also represented using a single heat kernel. In Figure 1(b) the evolution of the single heat kernels are given at time $t = 5$ with the exact solution. One may clearly observe that they approach to each other.

6.2. Initial approximations using many heat kernels

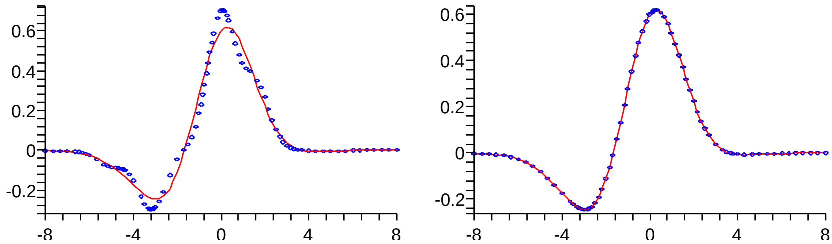
The high order asymptotic convergence in Theorem 3 indicates that $\varphi_n(x,t)$ is a good approximation of the solution $u(x,t)$ for all $t \geq 0$ if it gives a good initial approximation. In fact, the approximation showed an excellent behavior for $t > 1$ large in the numerical tests in [15]. However, the approximation showed poor behavior for $t \ll 1$ small. In the following test we mostly consider the initial approximation using backward moments with $t_0 > 0$. Also note that this initial approximation is not actually related to the heat equation. One may consider it as an approximation technique such as a Fourier integral.

6.2.1. Continuous initial values Consider the smooth initial value in (42) for the first example in this section. Using this initial value the backward heat equation can be solved up to backward time $t_0 = 1$. Hence one may say that the age of this initial value is 1, and it seems that taking backward time $t_0 = 1$ will give the best result. In Figure 2(a) an approximation using backward moment with the backward time $t_0 = 0.2$ and $n = 10$ is given. Its imaginary part was not taken in this example. One may observe a little bit of wiggling in this case. If the backward time approaches to the maximum backward time $t_0 = 1$, then the approximation agrees with the initial value completely. In Figure 2(b) an approximation with $t_0 = 0.4$ is given. Even if the backward time is increased to $t_0 = 4$, the initial approximation gives a perfect match.

The initial value for the second example is

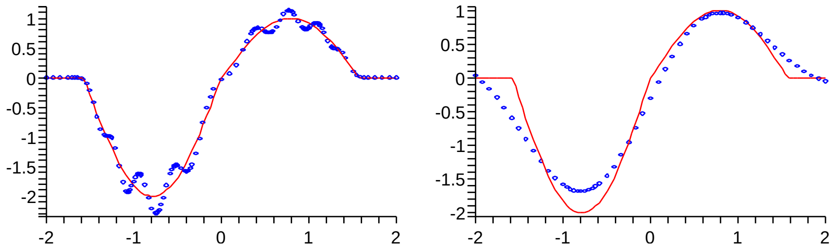
$$u_0(x) = \begin{cases} 2\sin(x)\,, & -\frac{\pi}{2} < x < 0, \\ \sin(x)\,, & 0 < x < \frac{\pi}{2}, \\ 0 \quad , & \text{otherwise}, \end{cases} \tag{43}$$

which is continuous, but not differentiable. Graphs of the approximations are given in Figure 3. The initial value $u_0(x)$ is given in (red) lines. Approximations obtained from moment problem using the real Hankel matrixes are given in (blue) dots. In Figure 3(a) a backward time $t_0 = 0.01$ is used. One may observe certain oscillations in the smooth regions. However, this approximation gives pretty correct approximation at the cusps.



(a) Initial approximation with $t_0 = 0.2$ (b) Initial approximation with $t_0 = 0.4$

Fig. 2. Initial approximations with $n = 10$ agrees very well if the age of the initial heat distribution is not zero and the backward time is close to it. In this example the age of the initial heat distribution is one.



(a) Initial approximation, $t_0 = 0.01$ (b) Initial approximation, $t_0 = 2.0$

Fig. 3. The initial value (43) is approximated using 10 heat kernels. The age of the initial heat distribution is zero. Only the region $x > 0$ is given.

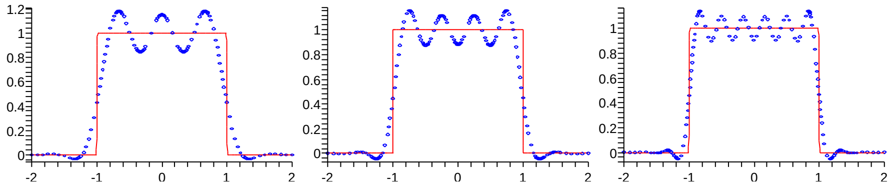
In Figure 3(b) a bigger backward time, $t_0 = 2.0$, is used. There is no oscillation at all for this case. However, it gives a poor approximation for the cusps. This approximation is too smooth to get it right. From this example, one may see that some parts of the initial value requires small backward time and other parts large ones. Hence it is desirable to develop a technique to give a freedom in choosing the backward time, say

$$\varphi_n(x,t) := Re\Big(\sum_{i=1}^{n} \frac{\rho_i}{\sqrt{4\pi(t+t_i)}}\, e^{-(x-c_i)^2/4(t+t_i)}\Big). \tag{44}$$

The technique in this paper is the case that all t_i's are fixed to be t_0. A back ward time $t_0 = 0.1$ gives better approximation for this example.

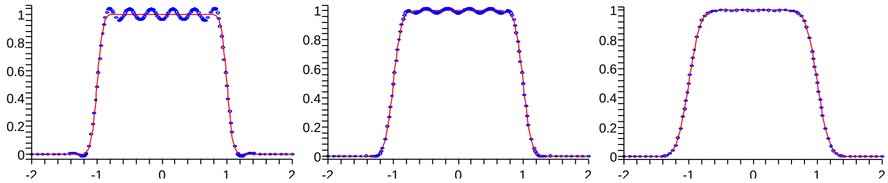
6.2.2. Discontinuous initial values Approximation of a discontinuous function gives extra difficulties. In this section we consider a discontinuous initial value

$$u_0(x) = \begin{cases} 1\,, & -1 < x < 1, \\ 0\,, & \text{otherwise.} \end{cases} \tag{45}$$



(a) $n = 10,\ t_0 = 0.2$ (b) $n = 20,\ t_0 = 0.2$ (c) $n = 40,\ t_0 = 0.2$

Fig. 4. Initial approximations of a discontinuous function show oscillations. The size of the oscillation is decreasing as $n \to \infty$.



(a) Solutions at $t = 0.0025$ (b) Solutions at $t = 0.005$ (c) Solutions at $t = 0.01$

Fig. 5. The initial oscillations disappear quickly. In this computation we set $n = 40$ and $t_0 = 0.2$. The exact solution and its approximation are given in lines and dots, respectively.

Then the solution $u(x,t)$ is given by

$$u(x,t) = \int_{-\infty}^{x} [\phi(y+1,t) - \phi(y-1,t)]dy. \tag{46}$$

In Figure 4 one may observe that the initial approximation has an oscillating behavior. In these examples a different kind of Gibb's phenomenon is observed. One can clearly see that the maximum error near the discontinuity is decreasing as n increases. The pattern of the oscillation is also different. However, in Figure 5, the oscillation disappears as time increases and the approximation agrees with the exact solutions completely at $t = 0.01$. One can also say that, if the initial value has regularity corresponding to the Figure 5(c), then the approximation using corresponding backward time gives a perfect initial match.

In Table 1 a comparison of the approximation error is given for four cases doubling the time from $t = 0.002$ to $t = 65.536$. Two node numbers of $n = 10$ and $n = 20$ and two backward times of $t_0 = 0.01$ and $t_0 = 0.2$ are compared. The errors are given in the uniform norm in the table. One can clearly observe the asymptotic convergence order given in Theorem 3. The convergence order at time $t > 0$ is computed using the following relation:

$$\text{asymptotic order} \cong \frac{\ln(\|u(t/2) - \varphi_n(t/2)\|_\infty / \|u(t) - \varphi_n(t)\|_\infty)}{\ln(1/2)}.$$

Table 1. The error in the table is given in L^∞-norms.

	$n = 10$, $t_0 = 0.01$		$n = 10$, $t_0 = 0.2$		$n = 20$, $t_0 = 0.01$		$n = 20$, $t_0 = 0.2$	
t	error	order	error	order	error	order	error	order
0.002	1.33e-01	0.34	2.65e-01	0.23	3.21e-03	0.22	9.53e-02	0.23
0.004	8.31e-02	0.68	1.94e-01	0.45	1.22e-03	1.39	6.93e-02	0.46
0.008	3.17e-02	1.39	1.05e-01	0.88	7.78e-05	3.97	3.66e-02	0.92
0.016	4.79e-03	2.73	3.28e-02	1.68	3.05e-07	7.99	1.03e-02	1.83
0.032	1.86e-04	4.69	4.00e-03	3.03	6.00e-11	12.31	8.85e-04	3.54
0.064	1.79e-06	6.70	1.40e-04	4.84	1.12e-15	15.71	1.21e-05	6.19
0.128	5.86e-09	8.25	1.38e-06	6.66	4.57e-21	17.90	1.69e-08	9.49
0.256	9.59e-12	9.25	4.95e-09	8.13	7.91e-27	19.14	2.23e-12	12.89
0.512	1.05e-14	9.84	8.76e-12	9.14	8.64e-33	19.80	4.01e-17	15.76
1.024	9.16e-18	10.16	1.01e-14	9.76	7.44e-39	20.15	1.76e-22	17.80
2.048	7.14e-21	10.33	9.07e-18	10.12	5.67e-45	20.32	3.26e-28	19.04
4.096	5.24e-24	10.41	7.18e-21	10.30	4.06e-51	20.41	3.71e-34	19.74
8.192	3.73e-27	10.46	5.31e-24	10.40	2.83e-57	20.46	3.27e-40	20.11
16.384	2.61e-30	10.48	3.80e-27	10.45	1.94e-63	20.48	2.53e-46	20.30
32.768	1.82e-33	10.49	2.67e-30	10.47	1.32e-69	20.49	1.83e-52	20.40
65.536	1.26e-36	10.49	1.86e-33	10.49	8.90e-76	20.49	1.27e-58	20.45

7. Conclusions

The moment problem for positive density functions has been generalized to complex density cases. This extended theory enabled us to solve a truncated moment problem for any real sequence by considering it as the real part of a complex moment problem. Finally, the approximation theory for the solutions to the heat equation is now complete for general sign-changing solutions and for $t > 0$ small using this extended theory. To obtain certain regularity in the initial approximation a method to use the backward moments has been developed. As a result we have obtained an approximation method for a function such as the Fourier integral.

There are many questions remaining related to this work. The construction $\varphi_n(x,t)$ depends on the choice of the density function $\varrho_0(x)$ and the backward time $t_0 > 0$. However, we do not have a criterion to choose a better density function $\varrho_0(x)$ and a better backward time t_0. It is conjectured that the complex moment problem (6) is solvable for all nontrivial $\varrho_0(x) \geq 0$. However, in Theorem 1, only the existence of a density function $\varrho_0(x)$ that gives the solvability of (6) is given. The geometric convergence order in (11) is observed numerically for the case with $t_0 = 0$ in [14]. It seems required to a more detailed numerical convergence test as $n \to \infty$ for the case with $t_0 > 0$. However, it is not given here since this paper is more focused on analysis. Analysis for the convergence as $n \to \infty$ seems a challenging problem.

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