Notes: Nevanlinna analytical Continuation Method

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Abstract

This is the abstract.

CONTENTS

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I. THE ANALYTIC CONTINUATION PROBLEM

The analytic continuation problem seeks to extract real frequency dynamical information from imaginary-time correlation functions $G(\tau)$ data. Technically, this is a highly nontirvial task[1]. To see this, we use the relation between $G(\tau)$ and $A(\omega)$ [1, 2]:

$$G(\tau) = \int_{-\infty}^{\infty} d\omega \frac{e^{-\tau\omega}}{1-\lambda e^{-\beta\omega}} A(\omega) = \int_{-\infty}^{\infty} d\omega K(\tau,\omega) A(\omega) \tag{1}$$

where $K(\tau,\omega) = \frac{e^{-\tau\omega}}{1-\lambda e^{-\beta\omega}}$ is the kernel, $\lambda = \pm 1$ for bosons/fermions respectively. One may consider to solve the problem by firstly discretize τ and ω and get:

$$G(\tau_i) = \sum_{j=1}^{N_\omega} K_{ij} A(\omega_j) \tag{2}$$

Then do SVD decomposition of rectangular matrix K, write $K_i j = U_{il}\lambda_l V_{lj}$. Finally the spectral function reads

$$A(\omega_j) = \sum_{l=1}^{N_\tau} \frac{1}{\lambda_l} V_{ij} \sum_{i=1}^{N_\omega} G(\tau_i) U_{il} \tag{3}$$

It seems fine at the first glanse. However, if we consider the properties of $K(\tau,\omega)$, we would notice that it is highly sigular since it is exponentially small for large $|\omega|$, so small errors $G(\tau)$ would be amplified by exponentially small λ_l. This problem is well-known ill-posed[3, 4] and enormous efforts have been made[].

II. HOW TO SOLVE?

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Here we introduce the recently developed Nevanlinna analytic continuation method[5].

III. NEVANLINNA ANALYTIC CONTINUATION METHOD

The Nevanlinna analytic continuation method[5] is an interpolation method. The key step is to build the conformal mappings from the open upper half of the complex plane $\mathcal{C}^+$ to a closed unit disk $\bar{\mathcal{D}}$ in the complex plane and make use of the Schur algorithm [6–8] to do the interpolate.

A. Schur Algorithm

Schur Algorithm was introduced by I. Schur[9] in Section 1 of Ref.[6]. Here we list the main results we need while for a detailed introduction, see Ref.[8].

A Schur class($\mathcal{S}$) consists of the Schur functions, which are the holomorphic functions from the open unit disk $\mathcal{D}$ to the closed unit disk $\bar{\mathcal{D}}$. For a given Schur function $s_0(z)$, the Schur algorithm defines a set of $\{s_j(z) \in \mathcal{S}\}_{0\leq j<\infty}$ starting from $s_0(z)$ by the recurrence relation:

$$zs_{j+1}(z) = \frac{s_j(z) - \gamma_j}{1 - \gamma_j^* s_j(z)} \tag{4}$$

where $s_j \in \mathcal{S}$ and $\gamma_j \equiv s_j(0)$ are called Schur parameters and $|\gamma_j| \leq 1$.

On the other hand, given an arbitrary strictly contractive sequence of Schur parameters $\{\gamma_0, \gamma_1, \ldots, \gamma_j, \ldots\} \subset \mathcal{D}$, one can construct a unique Schur function $s_0(z)$ by means of a continued fraction algorithm. In which we use the inverse relation of eq. (4)

$$s_j(z) = \frac{\gamma_j + zs_{j+1(z)}}{1 + \gamma_j^* z s_j(z)} \tag{5}$$

to construct the n-th Schur approximant, which we will denote by $s_0(z; \gamma_0, \gamma_1, \ldots, \gamma_n)$. Namely, we write:

$$s_n(z; \gamma_n) = \gamma_n \tag{6}$$

$$s_j(z; \gamma_j, \gamma_{j+1}, \ldots \gamma_n) = \frac{\gamma_j + zs_{j+1}(z; \gamma_{j+1}, \ldots \gamma_n)}{1 + \gamma_j^* z s_{j+1}(z; \gamma_{k+1}, \ldots \gamma_n)} \tag{7}$$

where $j = n-1, n-2, \ldots, 1, 0$.

Given the initial data consisting of N points $\{\mathcal{Y}_0, \mathcal{Y}_1, \ldots, \mathcal{Y}_{N-1}\} \subset \mathcal{D}$ and target data $\{\gamma_0, \gamma_1, \ldots, \gamma_{N-1}\} \subset \mathcal{D}$, we can find a holomorphic function $s(z) : \mathcal{D} \to \bar{\mathcal{D}}$ such that $s(\mathcal{Y}_j) = \gamma_j$ for all j by combining eq. (6), eq. (7) and the linear fractional transform $\xi(z, \mathcal{Y}_j) = \frac{z - \mathcal{Y}_j}{1 - z\mathcal{Y}_j^*}$:

$$s_{N-1}(z; \gamma_{N-1}) = \frac{\gamma_{N-1} + \xi(z, \mathcal{Y}_{N-1}) s_N(z)}{1 + \gamma_{N-1}^* \xi(z, \mathcal{Y}_{N-1}) s_N(z)} \tag{8}$$

$$s_j(z; \gamma_j, \gamma_{j+1}, \ldots \gamma_N) = \frac{\gamma_j + \xi(z, \mathcal{Y}_j) s_{j+1}(z; \gamma_{j+1}, \ldots \gamma_N)}{1 + \gamma_j^* \xi(z, \mathcal{Y}_j) s_{j+1}(z; \gamma_{k+1}, \ldots \gamma_N)} \tag{9}$$

where $j = N-2, N-3, \ldots, 1, 0$ and $s_0(z) \equiv s(z)$. In eq. (8), we notice that there is an degrees of freedom to choose an arbitrary $s_N(z) \in \mathcal{S}$, eq. (6) correponds the special case $s_{n+1}(z) = 0$.

G. Pick and R. Nevanlinna studied the interpolation problem independently in 1917[10] and 1919[11] respectively, showing that an interpolating function exists if and only if the Pick matrix

$$P_{jk} = \frac{1 - \gamma_k^* \gamma_j}{1 - \mathcal{Y}_j^* \mathcal{Y}_k} \tag{10}$$

is positive semi-definite. Furthermore, the function $s(z)$ is unique if and only if the Pick matrix has zero determinant. It is called the the Nevanlinna–Pick theorem.

B. Generalized Schur Algorithm

Schur algorithm can be modified to expand all contractive functions($\in \mathcal{B}$)[12], which are holomorphic functions mapping from the upper half plane $\mathcal{C}^+$ to $\bar{\mathcal{D}}$.

Given the initial data consisting of N points $\{\mathcal{Y}_0, \mathcal{Y}_1, \ldots, \mathcal{Y}_{N-1}\} \subset \mathcal{C}^+$ and target data $\{\gamma_0, \gamma_1, \ldots, \gamma_{N-1}\} \subset \bar{\mathcal{D}}$, in order to find a holomorphic function $\theta(z) \in \mathcal{B}$ such that $\theta(\mathcal{Y}_j) = z_j$ for all j, we should make use of the Mobius transform $h(z, \mathcal{Y}) = \frac{z-\mathcal{Y}}{z-\mathcal{Y}^*}$ which maps $\mathcal{C}^+/\bar{\mathcal{C}}^+$ to $\mathcal{D}/\bar{\mathcal{D}}$, which means it estabishes a one-to-one correspondence of $\theta(z)$ to a schur function $s(z)$ with:

$$\theta(h^{-1}(z, \mathcal{Y})) = s(z), \text{ or } \; s(h(z, \mathcal{Y})) = \theta(z) \tag{11}$$

We denote $h(z, \mathcal{Y}_j)$ as $h_j(z)$ form now on.

The recursion relation between $\theta_j(z)$ and the next contractive function $\theta_{j+1}(z)$ can be easily build as follows. From eq. (11), we have:

$$s_j(0) = \theta_j(h_j^{-1}(0)) = \theta_j(\mathcal{Y}_j) = \gamma_j \tag{12}$$

Let $\theta_{j+1}(z) = s_{j+1}(h_j(z))$, then use the recursion relation eq. (4), we have:

$$z\theta_{j+1}(h_j^{-1}(z)) = \frac{\theta_j(h_j^{-1}(z)) - \gamma_j}{1 - \gamma_j^* \theta_j(h_j^{-1}(z))} \stackrel{\text{def}}{=} \phi_j(h_j^{-1}(z)) \tag{13}$$

Form the first and the third terms of eq. (13) we have:

$$\phi_j(h_j^{-1}(z)) = z\theta_{j+1}(h_j^{-1}(z)) = h_j(h_j^{-1}(z))\theta_{j+1}(h_j^{-1}(z)) \tag{14}$$

replace $h_j^{-1}(z)$ with $z \in \mathcal{D}$ by $z \in \mathcal{C}^+$, we have

$$\phi_j(z) = h_j(z)\theta_{j+1}(z) \tag{15}$$

We can read from eq. (15) that $\phi_j(z) \in \mathcal{B}$ and $\phi_j(\mathcal{Y}_j) = 0$.

Form the second and the third terms of eq. (13) we can read:

$$\phi_j(z) = \frac{\theta_j(z) - \gamma_j}{1 - \gamma_j^* \theta_j(z)} \tag{16}$$

Together with eq. (15) we get the recursion relation between $\theta_j(z)$ and $\theta_{j+1}(z)$:

$$\theta_j(z) = \frac{\phi_j(z) + \gamma_j}{\gamma_j^* \phi_j(z) + 1} = \frac{h_j(z)\theta_{j+1}(z) + \gamma_j}{\gamma_j^* h_j(z)\theta_{j+1}(z) + 1} \tag{17}$$

The recursive final $\theta(z)$ can conveniently be written in a matrix form:

$$\theta(z)[z; \theta_N(z)] = \frac{a(z)\theta_N(z) + b(z)}{c(z)\theta_N(z) + d(z)} \tag{18}$$

where

$$\begin{pmatrix} a(z) & b(z) \\ c(z) & d(z) \end{pmatrix} = \prod_{j=1}^{N-1} \begin{pmatrix} h_j(z) & \gamma_j \\ \gamma_j^* h_j(z) & 1 \end{pmatrix} \tag{19}$$

with j increasing from left to right. Like in eq. (6), there is a alse freedom to choose $\theta_N(z)$.

C. Interpolation of Green's functions

The retared Green's function $G^R(\omega + i\eta)$ and the Masubara Green's function $G(i\omega_n)$ can be expressed consistently by replacing the variables $i\omega_n$ and $\omega + i\eta$ with a single complex variable z. $G(z)$ is analytic in the upper half plane $\mathcal{C}^+$. Our problem is that once we have Masubara frequencies $\{i\omega_n\} \subset \mathcal{C}^+$ and target data $\{G(i\omega_n)\} \subset \mathcal{C}$, where $\mathcal{C}$ is the complex plane, how can we get interpolate them and get the holomorphic function $G(z) : \mathcal{C}^+ \to C$?

Based on the knowledge of Schur algorithm, if we can find a one-to-one correspondence of $G(z)$ and a contractive function $\theta(z) \in \mathcal{B}$, then we can futher generalize the algorithm in section III B.

To do this, we firstly introduce the Nevanlinna functions $f(z) \in \mathcal{N}$. In complex analysis, a Nevanlinna function is a complex function that is analytic in the open upper half plane $\mathcal{C}^+$ and has non-negative imaginary part, i.e., maps into $\bar{\mathcal{C}}^+$ (the overline denotes inclusion of the boundary). The invertible Möbius transform $h(z) = \frac{z-i}{z+i}$ maps Nevanlinna functions one to one to contractive functions:

$$\theta(z) = h(f(z)), \text{ or } \; f(z) = h^{-1}(\theta(z)) \tag{20}$$

Given the initial data consisting of N points $\{\mathcal{Y}_0, \mathcal{Y}_1, \ldots, \mathcal{Y}_{N-1}\} \subset \mathcal{C}^+$ and target data $\{C_0, C_1, \ldots, C_{N-1}\} \subset \bar{\mathcal{C}}$, The only thing we needed is to let γ_j in eq. (17) be $\gamma_j \equiv h(C_j)$.

Moreover, the corresponding Pick matrix is generalized to:

$$P_{jk} = \frac{1 - h(C_k)^* h(C_j)}{1 - h(\mathcal{Y}_j)^* h(\mathcal{Y}_k)} \tag{21}$$

The aforementioned conformaling mappings are shown in fig. 1.

$$\begin{tikzcd}
\mathcal{C}^+ \arrow[r, "f"] \arrow[d, "h_j"'] \arrow[dr, "\theta"] & \bar{\mathcal{C}}^+ \arrow[d, "h"] \\
\mathcal{D} \arrow[r, "s"'] & \bar{\mathcal{D}}
\end{tikzcd}$$

f: Nevanlinna function $\in \mathcal{N}$

s: Schur function $\in \mathcal{S}$

θ: Contractive function $\in \mathcal{B}$

h/h_j: Conformal mapping

FIG. 1. Conformal mappings

Now we are ready to disscuss the Green's functions. The Lehmann representation of Green's function $G(z)$ is:

$$G(z) = \frac{1}{Z} \sum_{nm} |A_{nm}|^2 \frac{e^{-\beta E_n} \pm e^{-\beta E_m}}{z - E_m + E_n} \tag{22}$$

where the "+" sign is for fermionic Green's functions and "−" sign is for bosonic Green's functions.

In fermionic case, if we take $z = x + iy$ with $y > 0$, i.e. $z \in \mathcal{C}^+$, we can easily prove that $\mathrm{Im}G(z) \leq 0$. Therefore $-G(z) \in \mathcal{N}$ is an Nevanlinna function.

While the bosonic case is less trivial. The imaginary part of bosonic Green's function is:

$$\mathrm{Im}G(z) = \frac{1}{Z} \sum_{nm} \frac{y|A_{nm}|^2 e^{-\beta E_m}}{(x - E_m + E_n)^2 + y^2} [(1 - e^{\beta(E_m - E_n)}] \tag{23}$$

which is negative when $E_m > E_n$ and positive when $E_m < E_n$. We can construct a $\tilde{G}(z)$ like:

$$\tilde{G}(z) = \frac{1}{Z} \sum_{nm} \frac{|A_{nm}|^2}{z - E_m + E_n} \frac{e^{-\beta E_n} - e^{-\beta E_m}}{E_m - E_n} \tag{24}$$

and $-\tilde{G}(z) \in \mathcal{N}$ is a Nevanlinna function.

IV. HARDY BASIS OPTIMIZATION

Appendix A: Conformal transforms

1. The linear fractional transform

The linear fractional transform is:

$$\xi(z, \mathcal{Y}) = \frac{z - \mathcal{Y}}{1 - z\mathcal{Y}^*} \tag{A1}$$

It is a one to one mapping of the open unit disk $\mathcal{D}$ onto itself and a one to one mapping of the unit circle $\mathcal{T}$. It maps point $\mathcal{Y}$ to the center of $\mathcal{D}$.

2. The Mobius transform

The mapping from $\mathcal{C}^+/\bar{\mathcal{C}}^+$ to $\mathcal{D}^+/\bar{\mathcal{D}}^+$ is called Mobius transform. It has the form:

$$h(z, \mathcal{Y}) = \frac{z - \mathcal{Y}}{z - \mathcal{Y}^*} \tag{A2}$$

where $\mathcal{Y} \in \bar{\mathcal{C}}^+$ and $\mathcal{Y} \neq 0$. We can easily prove that $|h(z, \mathcal{Y})| \leq 1$ for $z \in \bar{\mathcal{C}}^+$ and $|h(z, \mathcal{Y})| = 1$ if z is real. $h(z, \mathcal{Y})$ maps $\mathcal{Y} \in \bar{\mathcal{C}}^+$ to the center of the unit disk $\mathcal{D}$ and the real axis as the edge of $\bar{\mathcal{D}}$, the rest part of upper half complex plane is wrapped inside the unit disk. If $\tilde{z} \in \mathcal{D}$, the inverse transform is:

$$h^{-1}(\tilde{z}, \mathcal{Y}) = \frac{\mathcal{Y} - \tilde{z}\mathcal{Y}^*}{1 - \tilde{z}} \tag{A3}$$

Angin one can prove $\mathrm{Im} h^{-1}(\tilde{z}, \mathcal{Y}) = (\mathrm{Im}\mathcal{Y})(1 - |\tilde{z}|^2) > 0$.

Proof of $|h(z, \mathcal{Y})| \leq 1$ for $z \in \bar{\mathcal{C}}^+$ and $|h(z, \mathcal{Y})| = 1$ if z is real. We already know that $\mathrm{Im}z \geq 0, \mathrm{Im}\mathcal{Y} > 0$.

$$\begin{aligned} |h(z, \mathcal{Y})|^2 &= \frac{z - \mathcal{Y}}{z - \mathcal{Y}^*}\frac{z^* - \mathcal{Y}^*}{z^* - \mathcal{Y}} = \frac{|z|^2 + |\mathcal{Y}|^2 - z\mathcal{Y}^* - z^*\mathcal{Y}}{|z|^2 + |\mathcal{Y}|^2 - z\mathcal{Y} - z^*\mathcal{Y}^*} \\ &= \frac{|z|^2 + |\mathcal{Y}|^2 - 2(\mathrm{Re}z\mathrm{Re}\mathcal{Y} + \mathrm{Im}z\mathrm{Im}\mathcal{Y})}{|z|^2 + |\mathcal{Y}|^2 - 2(\mathrm{Re}z\mathrm{Re}\mathcal{Y} - \mathrm{Im}z\mathrm{Im}\mathcal{Y})} \end{aligned} \tag{A4}$$

If $\mathrm{Im}z = 0$, $|h(z, \mathcal{Y})|^2 = 1$. If $\mathrm{Im}z > 0$, $|h(z, \mathcal{Y})|^2 < 1$. And we notice that if $\mathrm{Im}\mathcal{Y} = 0$, we map all points in $\bar{\mathcal{C}}$ to point 1 except for point $\mathcal{Y}$ itself.

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