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Implementation of the maximum entropy method for analytic continuation☆

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ABSTRACT

We present `Maxent`, a tool for performing analytic continuation of spectral functions using the maximum entropy method. The code operates on discrete imaginary axis datasets (values with uncertainties) and transforms this input to the real axis. The code works for imaginary time and Matsubara frequency data and implements the 'Legendre' representation of finite temperature Green's functions. It implements a variety of kernels, default models, and grids for continuing bosonic, fermionic, anomalous, and other data. Our implementation is licensed under GPLv3 and extensively documented. This paper shows the use of the programs in detail.

Program summary

Program Title: maxent

Program Files

doi: http://dx.doi.org/10.17632/rf3p4psdhs.1

Licensing provisions: GPLv3

Programming language: C++

Nature of problem: The analytic continuation of imaginary axis correlation functions to real frequency/time variables is an ill-posed problem which has an infinite number of solutions.

Solution method: The maximum entropy method obtains a possible solution that maximizes entropy, enforces sum rules, and otherwise produces 'smooth' curves. Our implementation allows for input in Matsubara frequencies, imaginary time, or a Legendre expansion. It implements a range of bosonic, fermionic and generalized kernels for normal and anomalous Green's functions, self-energies, and two-particle response functions.

External routines/libraries: ALPSCore [1][2], GSL, HDF5

[1] B. Bauer, et al., The ALPS project release 2.0: open source software for strongly correlated systems, J. Stat. Mech. Theor. Exp. 2011 (05) (2011) P05001. arXiv:1101.2646, doi:10.1088/17425468/2011/05/P05001.

[2] A. Gaenko, E. Gull, A.E. Antipov, L. Gamper, G. Carcassi, J. Paki, R. Levy, M. Dolfi, J. Greitemann, J.P.F. LeBlanc, Alpscore: Version 0.5.4doi: 10.5281/zenodo.50203.

1. Introduction

Analytic continuation of numerical data is a standard problem in condensed matter physics. It primarily appears when correlation functions of a many-body problem, computed in an imaginary time statistical mechanics formulation, need to be interpreted as response or spectral functions on the real axis. While imaginary time (or the Fourier transform, Matsubara frequency) correlation functions are naturally obtained in numerical simulations such

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as quantum Monte Carlo lattice [1] and impurity solvers [2–5], their real axis counterparts that correspond to response functions, which are measured in experiment, are not typically accessible to numerical techniques.

At the heart of this is that the continuation from the imaginary axis to the real axis is exceptionally ill conditioned, such that small fluctuations of the input data (either from statistical Monte Carlo noise or a truncation of the accuracy to finite precision numbers) lead to large fluctuations of the output data, rendering any direct transformations useless in practice. Several alternatives have been proposed, among them are the construction of rational polynomial functions (Padé approximants) [6–8], a constrained optimization procedure [9], a stochastic analytic continuation method [10], a stochastic regularization method [11,12], and a stochastic analytic inference method [13]. The standard method, however, is the so-called maximum entropy method (MEM) [14,15], for which we provide an implementation in this paper. A comparison between MEM and other methods for bosonic Green's functions has been studied in Ref. [16]. Our implementation, `Maxent`, is part of the ALPS applications [17–19] and makes use of the core ALPS libraries [20]. In the following, we will briefly review the formalism (referring the reader to Ref. [14] and the original literature for more details), introduce our implementation, and illustrate its usage with examples.

2. Analytic continuation

2.1. Analytic continuation formalism

We start our considerations with the imaginary time Green's function $G(\tau) = -\langle c(\tau)c^\dagger(0)\rangle$, which is a continuous function for $0 < \tau < \beta$, and is periodic for bosonic and anti-periodic for fermionic systems within $\tau \in [0, \beta]$. In this notation, c denotes an annihilation operator, $c^\dagger$ a creation operator, and the time-dependence of the operator and its expectation value are to be interpreted in the usual sense [21]. Imaginary time Green's functions of this type are the fundamental objects that most QMC methods produce as a simulation output. The Green's function in τ can be related to the Green's function on the imaginary frequency axis through a Fourier transform

$$G(i\omega_n) = \int_0^\beta e^{i\omega_n\tau} G(\tau). \tag{1}$$

The 'Matsubara' frequencies $i\omega_n$ come from poles of the distribution functions and are defined as $i\omega_n = 2\pi(n+\frac{1}{2})/\beta$ for fermionic and $i\omega_n = 2\pi n/\beta$ for bosonic operators.

For the rest of the article, we assume that these Green's functions are not known to arbitrary precision. Rather, we work with a truncation of the Green's function to N components, which are obtained by averaging a set of M estimates for each component, $G_n^{(i)}$, that are independent and Gaussian distributed so that if there are M samples for each n, the estimate for the Green's function is given by

$$G_n = \frac{1}{M}\sum_{j=1}^{M} G_n^{(j)}. \tag{2}$$

Different components n and m of the Green's function may be correlated. This is encapsulated in the covariance matrix C_{nm}, which is estimated as

$$C_{nm} = \frac{1}{M(M-1)}\sum_{j=1}^{M}(G_n - G_n^{(j)})(G_m - G_m^{(j)}). \tag{3}$$

In the case of fermions, the Matsubara frequency Green's function $G(i\omega_n)$ and its imaginary time counterpart $G(\tau)$ are related to a real frequency Green's function $G(\omega)$ via

$$G(i\omega_n) = \frac{-1}{\pi}\int_{-\infty}^{\infty}\frac{d\omega \mathrm{Im}\,[G(\omega)]}{i\omega_n - \omega}, \tag{4}$$

$$G(\tau_n) = \frac{1}{\pi}\int_{-\infty}^{\infty}\frac{d\omega \mathrm{Im}\,[G(\omega)]\, e^{-\tau_n\omega}}{1+e^{-\beta\omega}}, \tag{5}$$

where τ has been discretized in some manner to N points. The imaginary part of the Green's function that appears in the numerators of Eqs. (4) and (5) defines the spectral function

$$A(\omega) = -\frac{1}{\pi}\mathrm{Im}\,[G(\omega)]\,. \tag{6}$$

Obtaining $G(\omega)$ and $A(\omega)$ in addition to related quantities for bosonic and other response functions, as well as self-energies, is the main purpose of this paper.

We can formulate Eq. (5) as

$$G_n = G(\tau_n) = \int_{-\infty}^{\infty} d\omega\, A(\omega)K_n(\omega), \tag{7}$$

$$K_n(\omega) = K(\tau_n, \omega) = -\frac{e^{-\tau_n\omega}}{1+e^{-\omega\beta}}, \tag{8}$$

where K_n is the 'kernel' of the analytic continuation, here for a transformation of a fermionic Green's function from imaginary time to real frequencies. Kernels for other distribution functions and imaginary axis representations are listed in Section 3.3, Tables 3 and 4.

Given a candidate spectral function $A(\omega)$ on the real axis and the associated kernel, the imaginary axis Green's function can be evaluated using Eq. (7) to create an estimate $\bar{G}_n$, a process known as a back-continuation. To calculate the consistency of a spectral function $A(\omega)$ with the imaginary axis data G_n, one can define a "goodness of fit" quantity χ^2

$$\chi^2 = \sum_{n,m}^{M}(\bar{G}_n - G_n)^* C_{nm}^{-1}(\bar{G}_m - G_m), \tag{9}$$

where C_{nm} is defined in Eq. (3). Consistency of A with G_n within errors given by C_{nm} is achieved for $\chi^2 \sim M$. If the input data is uncorrelated then only the diagonal elements of the covariance matrix are non-zero, in which case χ^2 takes the form

$$\chi^2 = \sum_{n}^{M}\frac{(\bar{G}_n - G_n)^2}{\sigma_n^2} \tag{10}$$

where σ_n is the standard error in G_n.

2.2. Inversion of the kernel

To computationally solve for $A(\omega)$ in Eq. (7), the simplest method to employ is a least squares fitting routine, which attempts to minimize a functional $Q = \chi^2$ with χ^2 described in Eq. (9). While back-continuation is a straightforward procedure that gives a unique result, the inversion of Eq. (7) is ill conditioned, *i.e.* there are many solutions A that satisfy $G = KA$ to within the uncertainty given by C_{nm}.

2.3. Maximum entropy method

Instead of least-squares fitting, analytic continuation algorithms impose additional criteria on A, such as smoothness [9], in order to reduce the space of acceptable solutions. In the maximum entropy method an "entropy" term, S, is also considered to help regularize the solutions, such that the functional to minimize