Maxent Example - Bosonic Kernel

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Abstract

This document is part of a tutorial on the use of Maxent, a program for doing analytical continuation using the maximum entropy method. It will explain how to provide the program with the proper parameter file, data format for bosonic frequency data, and understand the output. This program uses the ALPSCore libraries[1, 2].

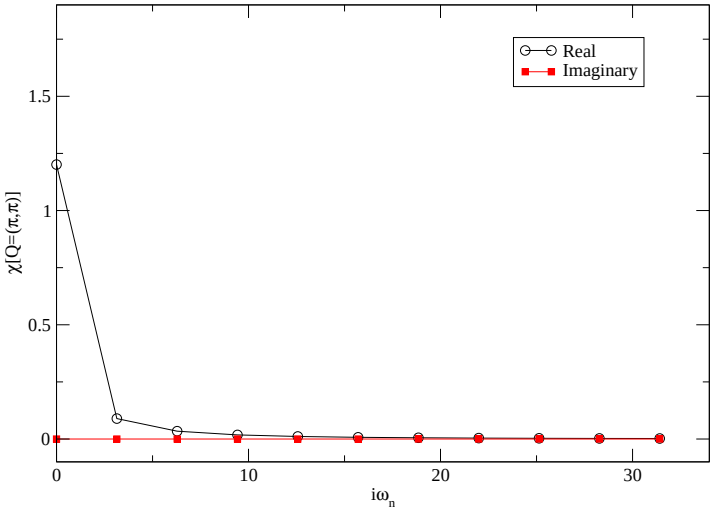
Contents

1 Introduction

Using DMFT and DCA with $U = 6$ and $\mu = -1.25$ ($n = 0.9$), we can generate the magnetic susceptibility χ of a 8-site Hubbard model with Hamiltonian

$$H = -\sum_{<ij>\sigma} t_{ij}\left(c^{\dagger}_{i\sigma}c_{j\sigma} + c^{\dagger}_{j\sigma}c_{i\sigma}\right) + U\sum_{i} n_{i\uparrow}n_{i\downarrow},$$

In particular, we will analytically continue the magnetic susceptibility at $Q = (\pi, \pi)$, which is shown below,



While this function is on the imaginary axis, we wish to analytically continue it to the real axis. Mathematically, this is equivalent to finding the spectral function $A(\omega) = \mathrm{Im}[\chi(\omega)] = \chi''(\omega)$ such that

$$\chi(i\omega_n) = \int_{-\infty}^{\infty} K(i\omega_n, \omega) A(\omega) d\omega,$$

with the kernel K written as $K(i\omega_n, \omega) = \dfrac{1}{i\omega_n + \omega}$ for this data. The Maxent procedure is one such method of determining $A(\omega)$.

2 File Structure

We've included several files that will be used to generate the remainder of this document:

Filenames and Descriptions

- *G_ im* = Im$[\chi(i\omega_n)]$
  - column format: $i\omega_n$ Im$[\chi(i\omega_n)]$ $\sigma_{I,n}$

Input file - G_im

```
0 -1.27890161453e-15 1.27890161453e-16
3.14159265359 4.895943813e-06 4.895943813e-07
6.28318530718 7.44279002171e-06 7.44279002171e-07
```

- *G_ re* = Re$[\chi(i\omega_n)]$
  - column format: $i\omega_n$ Re$[\chi(i\omega_n)]$ $\sigma_{R,n}$

Input file - G_re

```
0 1.20109669923 0.0001
3.14159265359 0.0894052697042 0.0001
6.28318530718 0.0342718849381 0.0001
```

- *dat_ in* = $\chi(i\omega_n)$ input format for Maxent
  - column format: $i\omega_n$ Re$[\chi(i\omega_n)]\sigma_{R,n}$ Im$[\chi(i\omega_n)]$ $\sigma_{I,n}$

Input file - dat_in

```
0 1.20109669923 0.0001 -1.27890161453e-15 1.27890161453e-16
3.14159265359 0.0894052697042 0.0001 4.895943813e-06 4.895943813e-07
6.28318530718 0.0342718849381 0.0001 7.44279002171e-06 7.44279002171e-07
```

3 Using Maxent

These files are easily used with Maxent. Here is the parameter file for this input

Param File bosonic.param

```
NORM = 1.20109669923            #the particular normalization for this data
OMEGA_MAX = 40                  #Spectral function is larger than default bounds
KERNEL = bosonic                #Using bosonic data
BETA = 2.0                      #inverse temperature
NFREQ = 1000                    #number of output frequencies
NDAT = 22                       #number of input data points*2 due to non-PH symmetry
MAX_IT = 4000                   #increase maximum iterations for convergence
DATASPACE = frequency           #frequency data
PARTICLE_HOLE_SYMMETRY = 0      #use both real and imag part of input
DATA=dat_in                     #name of data file
```

Using these parameters, specifically `PARTICLE_HOLE_SYMMETRY=0`, both the real and imaginary components of $\chi(i\omega_n)$ are read into Maxent, which is why for 11 complex data points `NDAT=22`. This data is also particle-hole symmetric, so one could treat the $\mathrm{Im}[\chi] = 0$ so that only the real data is input. This will not be shown here, but a sample parameter file is included, where `PARTICLE_HOLE_SYMMETRY=1` (with other necessary parameter changes).

Param File bosonic_ph.param

```
#this param file shows how the same data can be input with PH symmetry

NORM = 1.20109669923            #the particular normalization for this data
OMEGA_MAX = 40                  #Spectral function is larger than default bounds
KERNEL = bosonic                #Using bosonic data
BETA = 2.0                      #inverse temperature
NFREQ = 1000                    #number of output frequencies
NDAT = 11                       #actual number of input data points
MAX_IT = 4000                   #increase maximum iterations for convergence
DATASPACE = frequency           #frequency data
PARTICLE_HOLE_SYMMETRY = 1      #PH symmetric data; only real part
DATA=G_re                       #name of data file
```

3.1 Internal Kernel

While the expression for the spectral function of bosonic data is

$$\chi(i\omega_n) = \int d\omega \frac{A(\omega)}{i\omega_n + \omega},$$

when trying to determine $\omega = 0$ at $i\omega_n = 0$ we run into a problem. To fix this, we simply try to find $A(\omega)/\omega$ so that expression now reads:

$$\begin{aligned} \chi(i\omega_n) &= \int d\omega \frac{\omega}{i\omega_n + \omega} \cdot (A(\omega)/\omega) \\ &= \int d\omega \frac{\omega}{i\omega_n + \omega} \cdot B(\omega) \end{aligned}$$

The fitting routine then finds the normalized $A(\omega)/\omega$ and produces that and the proper output (see below).

3.2 Output Guide

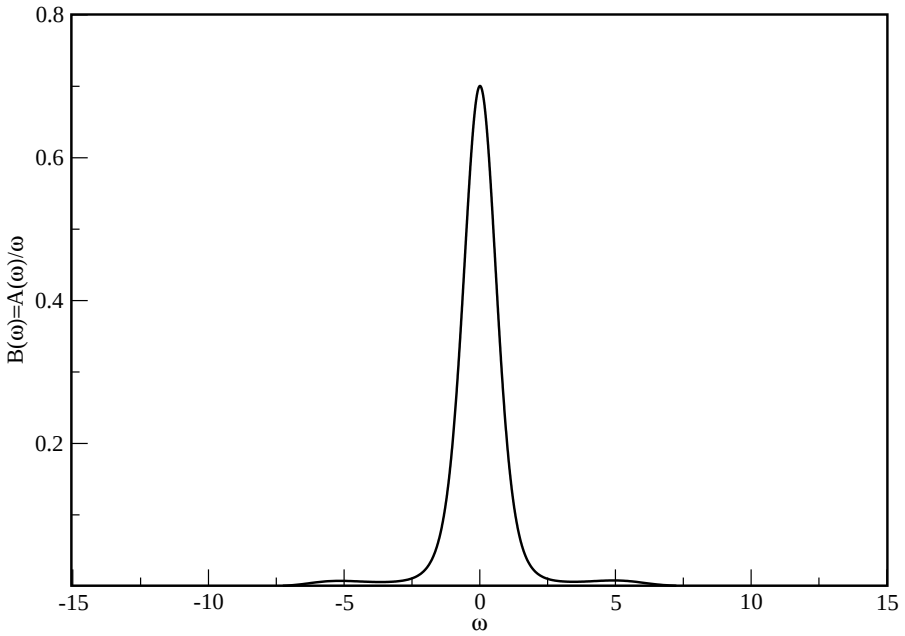
For the particular output of Maxent, please see the other example PDF files.

If text output is on, Maxent produces 13 files:

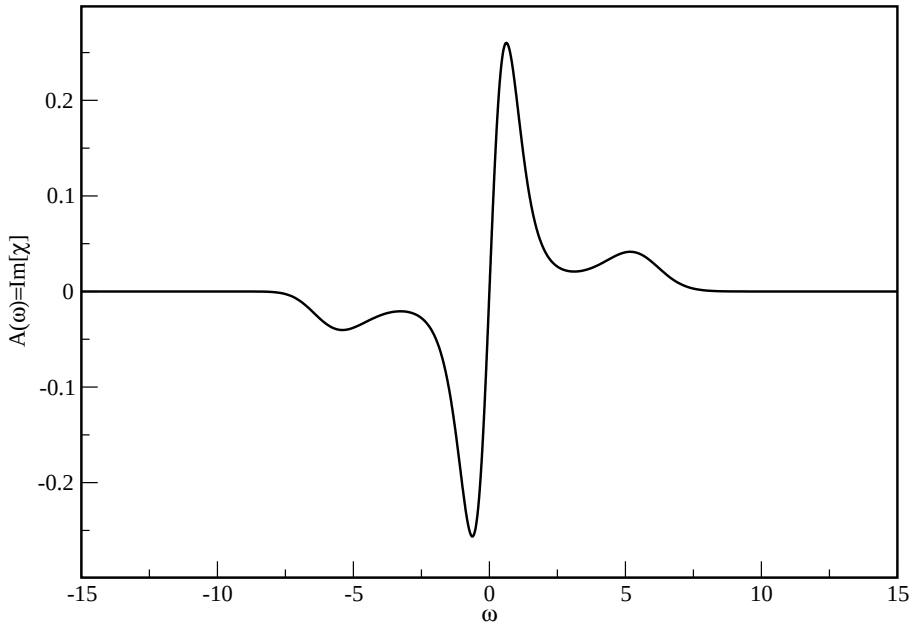
`name.out.avspec.dat`	Fitted spectral function (Imχ/ω) using Bayesian - **Bryan's method**
`name.out.avspec_back.dat`	The `avspec` spectrum continued back to the imaginary axis
`name.out.avspec_bose.dat`	$A(\omega) = \mathrm{Im}[\chi]$ with the proper sign and normalization; using **Bryan's method**
`name.out.chi2.dat`	Estimated χ^2 for each α value solution
`name.out.chispec.dat`	Spectral function satisfying the best χ^2 - **historic Maxent**
`name.out.chispec_back.dat`	The `chispec` spectrum continued back to the imaginary axis
`name.out.fits.dat`	Fits of each α value, see comments in file
`name.out.maxspec.dat`	Fitted spectral function (Imχ/ω) with the highest probability - **classic Maxent**
`name.out.maxspec_back.dat`	The `maxspec` spectrum continued back to the imaginary axis
`name.out.maxspec_bose.dat`	$A(\omega) = \mathrm{Im}[\chi]$ with the proper sign and normalization; using **classic Maxent**
`name.out.out.h5`	All output data in the hdf5 format
`name.out.prob.dat`	The posterior probability of each α value
`name.out.spex.dat`	All spectral functions produced; one for each α

For the xxspec files, the format of the data is ω $A(\omega)$ $d(\omega)$ where $d(\omega)$ is the default model.

In our example here is the "spectral" output $B(\omega) = A(\omega)/\omega$ from avspec:



while here is the proper spectral function $A(\omega)$ is found to be



It is important to note the kernel of the output, so that the proper back continuation can be performed. It is easiest to work with the xxspec.dat file so a frequency at $i\omega_n = 0$ can be generated as the true kernel (discussed in (3.1)) is singular.

References

[1] Alexander Gaenko, Emanuel Gull, Andrey E. Antipov, Lukas Gamper, Gabriele Carcassi, Joe Paki, Ryan Levy, Michele Dolfi, Jonas Greitemann, and James P. F. LeBlanc. ALPSCore: Version 0.5.4. April 2016. doi:10.5281/zenodo.50203.

[2] B Bauer et al. The ALPS project release 2.0: open source software for strongly correlated systems. *Journal of Statistical Mechanics: Theory and Experiment*, 2011(05):P05001, 2011. doi:10.1088/1742-5468/2011/05/P05001.