Maxent Example - Non-interacting Case

Ryan Levy
Physics Department, University of Michigan, Ann Arbor, MI

Abstract

This document is 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 particle-hole symmetric data (in both τ and $i\omega_n$), and understand the output. This program uses the ALPSCore libraries[1, 2].

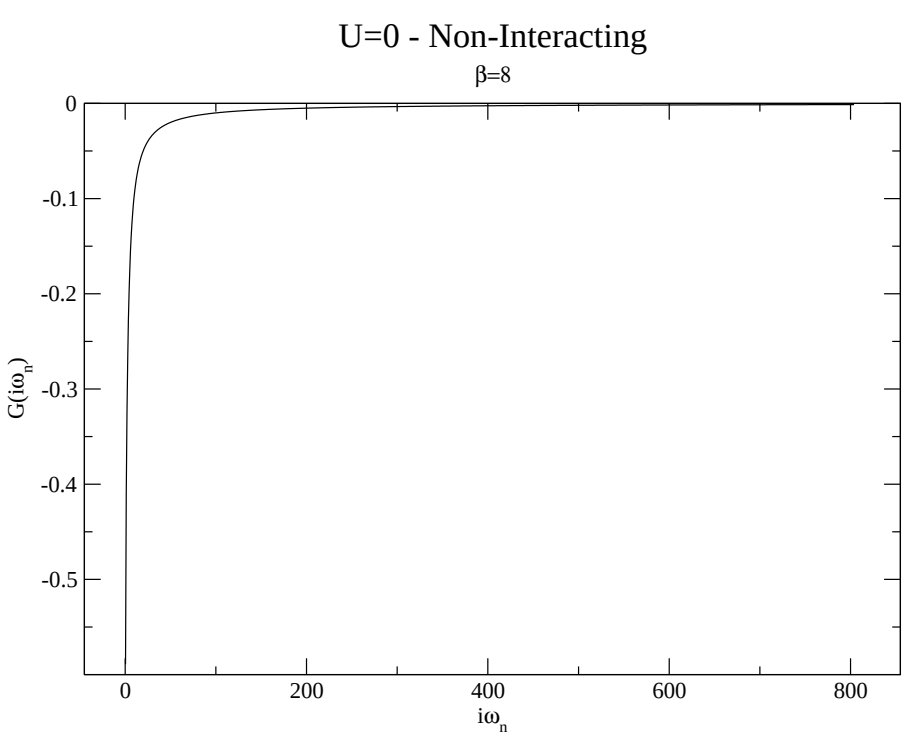
Contents

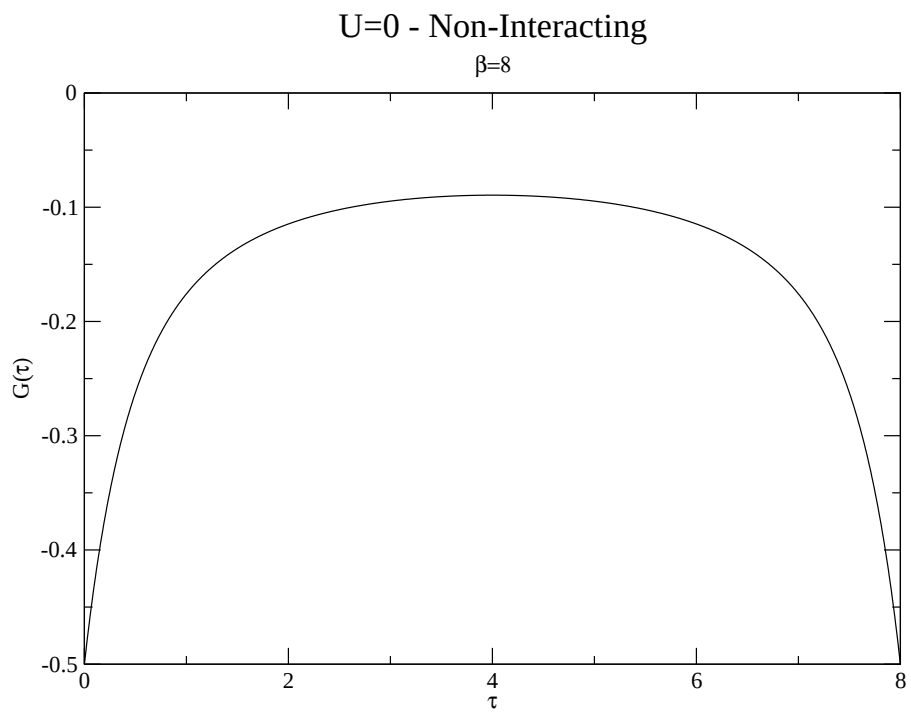
1 Introduction

Using DMFT we can set $U = 0$ and generate the non-interacting Hubbard model

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

This produces a Green's function in Matsubara space and Time space:


U=0 - Non-Interacting
β=8
0
-0.1
-0.2
-0.3
-0.4
-0.5
G(iω_n)
0
200
400
600
800
iω_n


U=0 - Non-Interacting
β=8
0
-0.1
-0.2
-0.3
-0.4
-0.5
G(τ)
0
2
4
6
8
τ

While these functions are on the imaginary axis, we wish to analytically continue them to the real axis. Mathematically, this is equivalent to finding the spectral function $A(\omega) = -\frac{1}{\pi}\text{Im}[G(\omega)]$ such that

$$G(X) = \int_{-\infty}^{\infty} K(X,\omega)A(\omega)d\omega,$$

with the kernel K written as $K(i\omega_n,\omega) = \frac{1}{i\omega_n - \omega}$ or $K(\tau,\omega) = \frac{-e^{-\tau\omega}}{1+e^{-\omega\beta}}$ 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$[G(i\omega_n)]$, also input format for maxent
  - column format: $i\omega_n$ Im$[G(i\omega_n)]$ $\sigma_{I,n}$

Input file - G_im

```
0.39269908169872 -0.58900239090596 1e-05
1.1780972450962 -0.40986302909581 1e-05
1.9634954084936 -0.32440959736089 1e-05
```

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

Input file - G_re

```
#Freq 0 1e-05
0.39269908169872 4.1987536135299e-16 1e-05
1.1780972450962 2.1665780666625e-16 1e-05
```

- *Gtau* = $G(\tau)$, also input format for maxent
  - column format: τ $G(\tau)$ σ_τ

Input file - Gtau

```
0 -0.5 1e-05
0.0078125 -0.49377185389756 1e-05
0.015625 -0.48766306852771 1e-05
```

3 Using Maxent

These files are easily used with Maxent. Here is the frequency space input file:

Param File in.param

```
BETA=8                    #inverse temperature
NDAT=1024                 #num of data points
NFREQ=500                 #num of output frequencies
DATASPACE=frequency       #G(iω)
KERNEL=fermionic           #fermionic/bosonic values
PARTICLE_HOLE_SYMMETRY=1  #0/1
DATA="G_im"                #location of data file
```

Maxent then produces the following output:

Maxent output

```
./maxent in.param
Using flat default model
using kernel fermionic in domain frequency with ph symmetry
Kernel is set up
# 0     6.27911e+06
# 1     1.16635e+06
# 2     258981
# 3     68739
# 4     17040.5
# 5     3761.79
# 6     744.024
# 7     132.167
minimal chi2: 2.55387e-05
alpha it: 0     WARNING: iteration reached max_it without converging, your
    minimizer is having problems. Please be careful!
Q = 0.5chi^2-\alpha*entropy: 987272     norm: 1.034
alpha it: 1     WARNING: iteration reached max_it without converging, your
    minimizer is having problems. Please be careful!
Q = 0.5chi^2-\alpha*entropy: 155.23     norm: 1.00046
alpha it: 2     Q = 0.5chi^2-\alpha*entropy: 93.5       norm: 1.00035
alpha it: 3     Q = 0.5chi^2-\alpha*entropy: 82.1164    norm: 1.00033
alpha it: 4     Q = 0.5chi^2-\alpha*entropy: 72.0799    norm: 1.0003
....                            .....                  .....
alpha it: 55    Q = 0.5chi^2-\alpha*entropy: 0.0395693  norm: 1.00001
alpha it: 56    Q = 0.5chi^2-\alpha*entropy: 0.0337866  norm: 1.00001
alpha it: 57    Q = 0.5chi^2-\alpha*entropy: 0.028796   norm: 1
alpha it: 58    Q = 0.5chi^2-\alpha*entropy: 0.0245097  norm: 1
alpha it: 59    Q = 0.5chi^2-\alpha*entropy: 0.0208447  norm: 1
Ng: 7.3691
chi2 max: 3.66901
posterior probability of the default model: 1.59791e-24
```

3.1 Time input file

The input file for $G(\tau)$ can be slightly more complex. You can either supply the tau grid points through the parameter file or input file, with the param file used over input. An example of such a param file is included:

Param File in_tau.param

```
BETA=8                      #inverse temperature
NDAT=1025                   #num of data points
NFREQ=500                   #num of output frequencies;
KERNEL=fermionic             #fermionic/bosonic values
PARTICLE_HOLE_SYMMETRY=1    #0/1
DATASPACE=time               #G(τ)
DATA="Gtauin"                #location of data file
TAU_0=0.0
TAU_1=0.0078125
```

Using your own τ input generates a message confirming the choice of τ grid:

```
Using flat default model
using kernel fermionic in domain time with ph symmetry
Using param input tau points
Kernel is set up
```

When τ grid data is solely used from an input file, Maxent reads `Using data file tau points`

3.2 Output Guide

```
Using flat default model
using kernel fermionic in domain frequency with ph symmetry
Kernel is set up
```

These are the setup messages, confirming your input choices.

```
# 0 6.27911e+06
# 1 1.16635e+06
# 2 258981
# 3 68739
# 4 17040.5
# 5 3761.79
# 6 744.024
# 7 132.167
minimal chi2: 2.55387e-05
```

These represent the eigenvalues that are above precision after the single value decomposition (SVD). The last line represents the smallest χ^2 value the program thinks it will achieve. If this is $\gg 1$ there may be something wrong with your input

```
...
alpha it: 2 Q = 0.5chi^2-\alpha*entropy: 93.5 norm: 1.00035
alpha it: 3 Q = 0.5chi^2-\alpha*entropy: 82.1164 norm: 1.00033
...
```

The root finding procedure will print the iterations through α values in the range given by the parameters (default: 60 values $\in [0.01, 20]$) If the first two or three do not minimize properly that is ok, as long as the rest continue normally. Notice that the norm stays $\approx$1 for all iterations

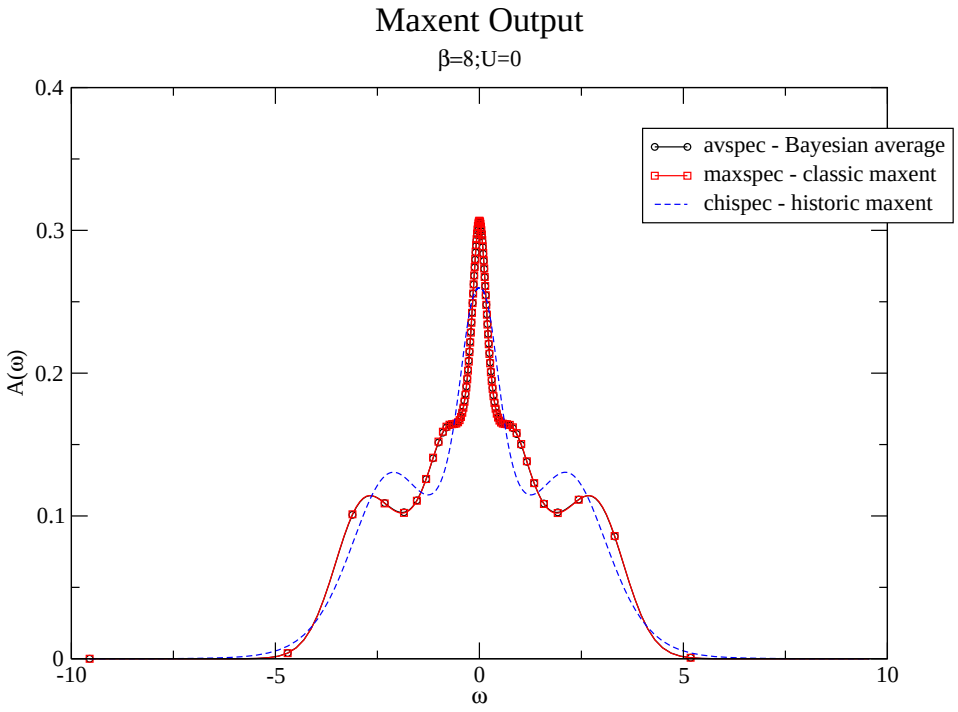
```
Ng: 7.3691
chi2 max: 3.66901
posterior probability of the default model: 1.59791e-24
```

This is posted after completing all α values and root finding. Ng represents the number of "good input points," chi2 max is the maximum value of χ^2 in the α iterations, and the last line is the probability that the default model is the correct representation of the spectral function. Note that that posterior probability has no normalization.

If text output is on, Maxent produces 8 files:

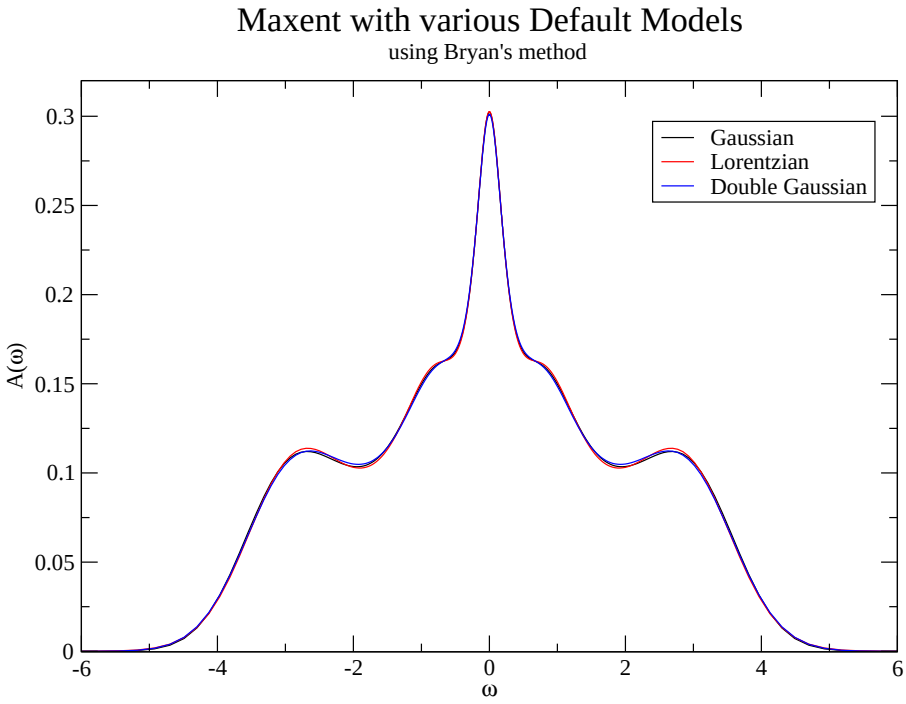
`name.out.avspec.dat`	Spectral function using Bayesian Averaging - **Bryan's method**
`name.out.chi2.dat`	Estimated χ^2 for each α value solution
`name.out.chispec.dat`	Spectral function satisfying the best χ^2 - **historic Maxent**
`name.out.fits.dat`	Fits of each α value, see comments in file
`name.out.maxspec.dat`	Spectral function with the highest probability - **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

In our example here are the spectral outputs:



4 Fine-Tuning Output

Different default models shouldn't change the results much, but sometimes end up doing so. One must be wary not to use a default model whose entropy is too 'strong' so that Maxent gets stuck in that local minimum. Here are a variety of models from the above example:



With $\sigma = 1, \Gamma = 0.5, \mu(\text{shift}) = 2$. This represents well behaved data within Maxent.

References

[1] Alexander Gaenko, Emanuel Gull, Andrey E. Antipov, Lukas Gamper, and Gabriele Carcassi. ALPSCore: Version 0.4.5. May 2015. doi:10.5281/zenodo.17398.

[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.