Maxent Example - Self-Energy of an Insulator

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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 of a self-energy in Matsubara space, and understand the output. Included as a supplement is the corresponding interacting Green's function input data. The data provided is of an interacting Hubbard model with $U = 10$, $\beta = 2$ for 1 site at half filling. This program uses the ALPSCore libraries[1, 2].

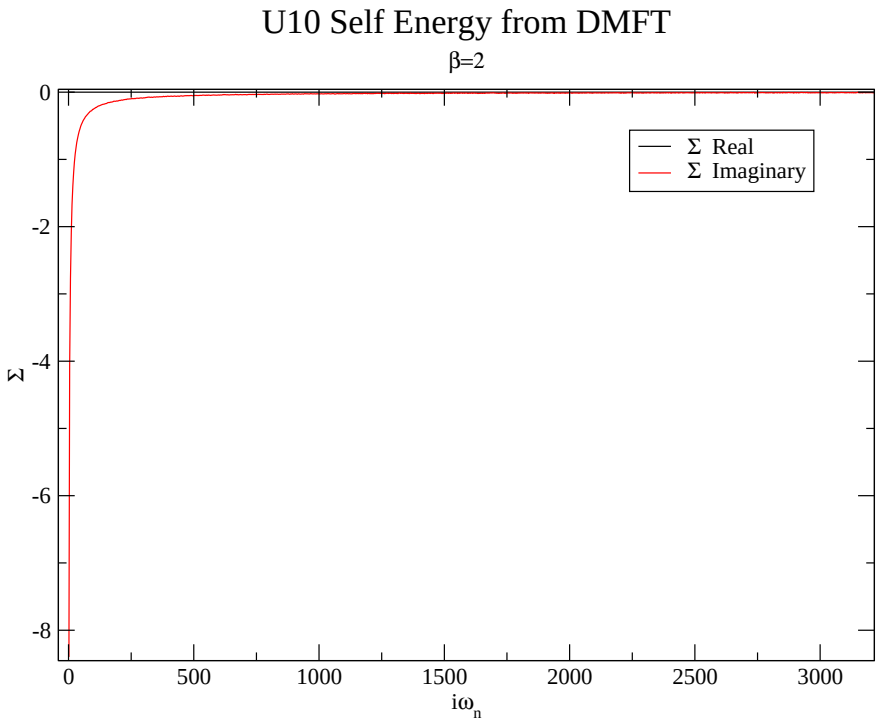
Contents

1 Introduction

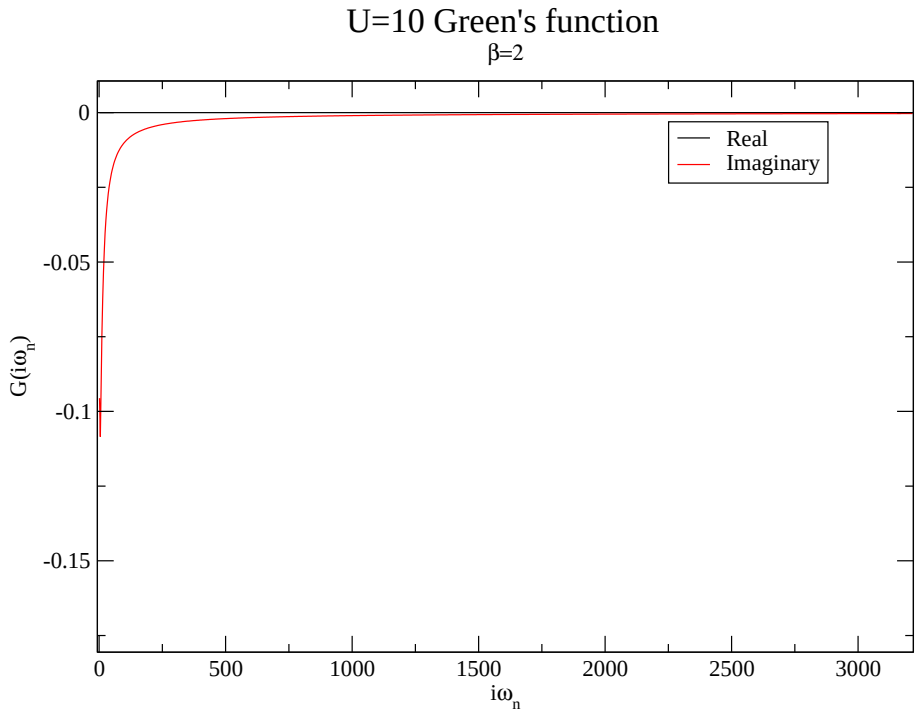
Using DMFT we can set $U = 10$ for a single site at half-filling to generate the interacting Hubbard model

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

This produces a self-energy output in Matsubara space:



Measured separately is the Green's function:



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 $A(\omega) = \mathrm{Im}[\Sigma(\omega)]$ such that

$$G(X) = -\frac{1}{\pi}\int_{-\infty}^{\infty} K(X,\omega)A(\omega)d\omega,$$

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

1.1 Normalization

Note that unlike a Green's function, the normalization (aka high frequency term) is not 1. For a self energy:

$$\Sigma = \Sigma_0 + \frac{\Sigma_1}{i\omega_n} + \dots$$

where $\Sigma_0 = Un$ (known as the Hartree term) and $\Sigma_1 = U^2 n(1-n)$[3]. This normalization is important to Maxent, as it is assumed to be the Green's function normalization of 1. For $U = 10$, there is a normalization of 25.

1.2 Errors

In this case, DMFT self-energies are lacking error bars. Since errors go like $\dfrac{1}{\sqrt{N}}$ where N is the number of samples, we can instead use this as an order of magnitude estimate for the error. This data had 2795305 sample iterations, and we therefore choose an estimated error $\sigma = 0.0006$

2 File Structure

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

Filenames and Descriptions

- *Selfenergy* = $\Sigma(i\omega_n)$ data values
  - column format: $i\omega_n$ Re$[\Sigma(i\omega_n)]$ Im$[G(i\omega_n)]$

Input file - Selfenergy

```
1.5707963267949  -1.77090655595753e-06  -8.3974060699946
4.7123889803847  -4.63021232511973e-07  -4.0755126985707
7.8539816339745  -1.04016996106358e-07  -2.7651531707533
```

- *Selfin* = $\Sigma(i\omega_n)$ input format for Maxent
  - column format: $i\omega_n$ $Im[G(i\omega_n)]$ $\sigma_{I,n}$

Input file - Selfin

```
1.5707963267949  -8.3974060699946  0.0006
4.7123889803847  -4.0755126985707  0.0006
7.8539816339745  -2.7651531707533  0.0006
```

- *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

```
1.5707963267949  -0.095565345664949  0.0006
4.7123889803847  -0.10849052589814  0.0006
7.8539816339745  -0.091077386535211  0.0006
```

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

Input file - G_re

```
1.5707963267949  2.6971654273943e-08  0.0006
4.7123889803847  1.1051970372948e-08  0.0006
7.8539816339745  2.1579065365108e-09  0.0006
```

3 Using Maxent

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

Param File in.param

```
BETA=2                        #inverse temperature
NDAT=1024                     #num of data points
NFREQ=500                     #num of output frequencies
DATASPACE=frequency           #G(iω)
KERNEL=fermionic              #fermionic/bosonic values
FREQUENCY_GRID=Quadratic      #this grid is better for features away from 0
PARTICLE_HOLE_SYMMETRY=1      #0/1
DATA="Selfin"                 #location of data file
SELF=1                        #this will output Σ(ω) rather than A(ω)
NORM=25                       #self energy norm = U^2 · n(1 − n)
```

Maxent then produces the following output:

Maxent output

```
Using flat default model
using kernel fermionic in domain frequency with ph symmetry
The high frequency limit is not 1!: 0.939857 Check norm?
Kernel is set up
# 0     347816
# 1     105909
# 2     20135.3
# 3     2450.83
# 4     202.67
# 5     11.8002
minimal chi2: 11.9801
WARNING: Redefinition of parameter NORM: Input (and output) data are assumed to be
     normalized to NORM.
alpha it: 0     WARNING: iteration reached max_it without converging, your
    minimizer is having problems. Please be careful!
Q = 0.5chi^2-\alpha*entropy: 6838.39    norm: 1.00725
alpha it: 1     Q = 0.5chi^2-\alpha*entropy: 6245.61    norm: 1.00245
alpha it: 2     Q = 0.5chi^2-\alpha*entropy: 6232.89    norm: 1.0023
alpha it: 3     Q = 0.5chi^2-\alpha*entropy: 6221.21    norm: 1.00216
alpha it: 4     Q = 0.5chi^2-\alpha*entropy: 6210.58    norm: 1.00202
alpha it: 5     Q = 0.5chi^2-\alpha*entropy: 6201       norm: 1.00189
alpha it: 6     Q = 0.5chi^2-\alpha*entropy: 6192.46    norm: 1.00176
alpha it: 7     Q = 0.5chi^2-\alpha*entropy: 6184.9     norm: 1.00164
alpha it: 8     Q = 0.5chi^2-\alpha*entropy: 6178.27    norm: 1.00153
alpha it: 9     Q = 0.5chi^2-\alpha*entropy: 6172.52    norm: 1.00142
alpha it: 10    Q = 0.5chi^2-\alpha*entropy: 6167.56    norm: 1.00132
alpha it: 11    Q = 0.5chi^2-\alpha*entropy: 6163.31    norm: 1.00123
alpha it: 12    Q = 0.5chi^2-\alpha*entropy: 6159.71    norm: 1.00114
alpha it: 13    Q = 0.5chi^2-\alpha*entropy: 6156.67    norm: 1.00106
alpha it: 14    Q = 0.5chi^2-\alpha*entropy: 6154.11    norm: 1.00098
alpha it: 15    Q = 0.5chi^2-\alpha*entropy: 6151.97    norm: 1.00091
alpha it: 16    Q = 0.5chi^2-\alpha*entropy: 6150.19    norm: 1.00085
alpha it: 17    Q = 0.5chi^2-\alpha*entropy: 6148.71    norm: 1.00079
alpha it: 18    Q = 0.5chi^2-\alpha*entropy: 6147.47    norm: 1.00074
alpha it: 19    Q = 0.5chi^2-\alpha*entropy: 6146.44    norm: 1.00069
alpha it: 20    Q = 0.5chi^2-\alpha*entropy: 6145.57    norm: 1.00065
alpha it: 21    Q = 0.5chi^2-\alpha*entropy: 6144.84    norm: 1.00061
alpha it: 22    Q = 0.5chi^2-\alpha*entropy: 6144.21    norm: 1.00057
alpha it: 23    Q = 0.5chi^2-\alpha*entropy: 6143.67    norm: 1.00053
alpha it: 24    Q = 0.5chi^2-\alpha*entropy: 6143.19    norm: 1.0005
alpha it: 25    Q = 0.5chi^2-\alpha*entropy: 6142.77    norm: 1.00047
alpha it: 26    Q = 0.5chi^2-\alpha*entropy: 6142.38    norm: 1.00045
alpha it: 27    Q = 0.5chi^2-\alpha*entropy: 6142.02    norm: 1.00042
```

```
alpha it: 28    Q = 0.5chi^2-\alpha*entropy: 6141.68    norm: 1.00039
alpha it: 29    Q = 0.5chi^2-\alpha*entropy: 6141.35    norm: 1.00037
alpha it: 30    Q = 0.5chi^2-\alpha*entropy: 6141.03    norm: 1.00035
alpha it: 31    Q = 0.5chi^2-\alpha*entropy: 6140.72    norm: 1.00033
alpha it: 32    Q = 0.5chi^2-\alpha*entropy: 6140.41    norm: 1.0003
alpha it: 33    Q = 0.5chi^2-\alpha*entropy: 6140.1     norm: 1.00028
alpha it: 34    Q = 0.5chi^2-\alpha*entropy: 6139.79    norm: 1.00026
alpha it: 35    Q = 0.5chi^2-\alpha*entropy: 6139.49    norm: 1.00024
alpha it: 36    Q = 0.5chi^2-\alpha*entropy: 6139.19    norm: 1.00022
alpha it: 37    Q = 0.5chi^2-\alpha*entropy: 6138.89    norm: 1.0002
alpha it: 38    Q = 0.5chi^2-\alpha*entropy: 6138.6     norm: 1.00018
alpha it: 39    Q = 0.5chi^2-\alpha*entropy: 6138.32    norm: 1.00016
alpha it: 40    Q = 0.5chi^2-\alpha*entropy: 6138.04    norm: 1.00014
alpha it: 41    Q = 0.5chi^2-\alpha*entropy: 6137.78    norm: 1.00013
alpha it: 42    Q = 0.5chi^2-\alpha*entropy: 6137.53    norm: 1.00011
alpha it: 43    Q = 0.5chi^2-\alpha*entropy: 6137.29    norm: 1.00009
alpha it: 44    Q = 0.5chi^2-\alpha*entropy: 6137.06    norm: 1.00007
alpha it: 45    Q = 0.5chi^2-\alpha*entropy: 6136.85    norm: 1.00005
alpha it: 46    Q = 0.5chi^2-\alpha*entropy: 6136.65    norm: 1.00004
alpha it: 47    Q = 0.5chi^2-\alpha*entropy: 6136.47    norm: 1.00002
alpha it: 48    Q = 0.5chi^2-\alpha*entropy: 6136.3     norm: 1
alpha it: 49    Q = 0.5chi^2-\alpha*entropy: 6136.15    norm: 0.99999
alpha it: 50    Q = 0.5chi^2-\alpha*entropy: 6136.01    norm: 0.999975
alpha it: 51    Q = 0.5chi^2-\alpha*entropy: 6135.88    norm: 0.999961
alpha it: 52    Q = 0.5chi^2-\alpha*entropy: 6135.77    norm: 0.999947
alpha it: 53    Q = 0.5chi^2-\alpha*entropy: 6135.66    norm: 0.999934
alpha it: 54    Q = 0.5chi^2-\alpha*entropy: 6135.57    norm: 0.999922
alpha it: 55    Q = 0.5chi^2-\alpha*entropy: 6135.49    norm: 0.99991
alpha it: 56    Q = 0.5chi^2-\alpha*entropy: 6135.42    norm: 0.999899
alpha it: 57    Q = 0.5chi^2-\alpha*entropy: 6135.35    norm: 0.999889
alpha it: 58    Q = 0.5chi^2-\alpha*entropy: 6135.3     norm: 0.999879
alpha it: 59    Q = 0.5chi^2-\alpha*entropy: 6135.25    norm: 0.999869
Ng: 5.25019
posterior probability of the default model: 0
spectra     max backcont diff     chi^2 value
=======     =================     ===========
chispec         0.000281127          12270.5
avspec          0.000281213          12282.9
maxspec         0.000281205          12281.7
```

3.1 Output Guide

```
Using flat default model
using kernel fermionic in domain frequency with ph symmetry
The high frequency limit is not 1!: 0.939857 Check norm?
Kernel is set up
```

These are the setup messages, confirming your input choices. There is a warning for the high frequency limit, but because our data is very noisy it can be ignored. If this limit was significantly off from 1, then your input NORM should be confirmed.

```
# 0 347816
# 1 105909
# 2 20135.3
# 3 2450.83
# 4 202.67
# 5 11.8002
minimal chi2: 11.9801
```

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 or it is very noisy

```
...
alpha it: 2 Q = 0.5chi^2-\alpha*entropy: 6232.89 norm: 1.0023
alpha it: 3 Q = 0.5chi^2-\alpha*entropy: 6221.21 norm: 1.00216
...
```

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: 5.25019
chi2 max: 12281.7
posterior probability of the default model: 0
```

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 known normalization.

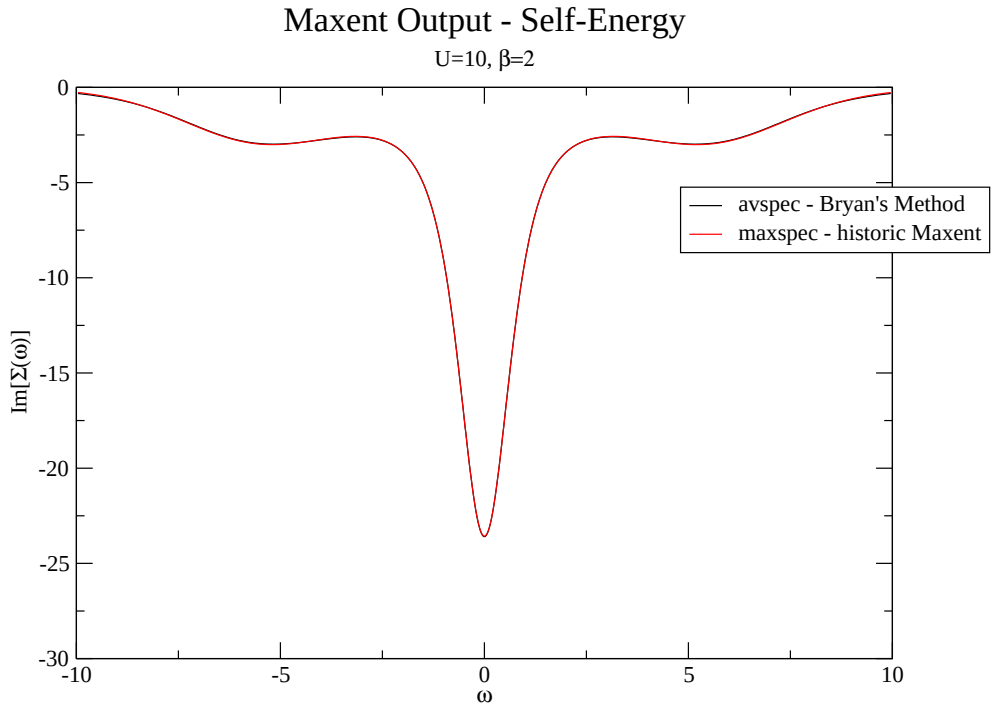
```
spectra     max backcont diff    chi^2 value
=======     =================    ===========
chispec        0.000281127          12270.5
avspec         0.000281213          12282.9
maxspec        0.000281205          12281.7
```

By default, maxent will back-continue, or continue back to the imaginary axis, the spectral function maxent output. Here two useful values are shown, the maximum difference between any of the back-continued points and input data, as well as the χ^2 value.

If text output is on, Maxent produces 13 files:

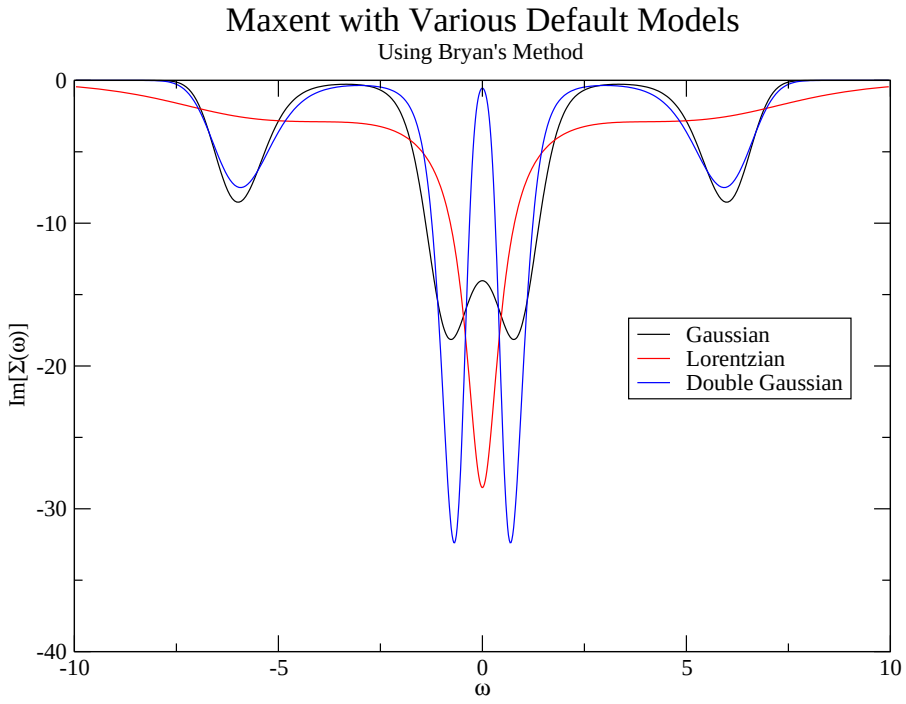
name.out.avspec.dat	"Spectral function" using Bayesian Averaging - **Bryan's method**
name.out.avspec_back.dat	The avspec spectrum continued back to the imaginary axis
name.out.avspec_self.dat	Im[$\Sigma(\omega)$] with the proper sign and normalization; using **Bryan's method**
name.out.chi2.dat	Estimated 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	"Spectral function" with the highest probability - **classic Maxent**
name.out.maxspec_back.dat	The maxspec spectrum continued back to the imaginary axis
name.out.maxspec_self.dat	Im[$\Sigma(\omega)$] 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

Because this is a self-energy, Maxent treats the input as a Green's function and finds a spectral function associated with it, but the spectral function output itself is meaningless. In our example here are the self-energy outputs with a flat default model:



4 Fine-Tuning Output

Different default models shouldn't change the results much, but sometimes end up doing so. Here are a variety of models from the above example:



With $\sigma = 0.5, \Gamma = 0.5, \mu(\text{shift}) = 4$. Notice that when given a Lorentzian default model, Maxent gets stuck into a local minimum similar to the flat model. After providing a Gaussian, Maxent finds structure away from the origin, which is then confirmed with the double Gaussian default model.

References

[1] 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.

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

[3] Xin Wang, Emanuel Gull, Luca de' Medici, Massimo Capone, and Andrew J. Millis. Antiferromagnetism and the gap of a mott insulator: Results from analytic continuation of the self-energy. *Phys. Rev. B*, 80:045101, Jul 2009. URL: http://link.aps.org/doi/10.1103/PhysRevB.80.045101, doi:10.1103/PhysRevB.80.045101.