Maxent Example - Self-Energy of a Metal

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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 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 $U = 1, \beta = 2$ for 1 site at half filling. This program uses the ALPSCore libraries[1, 2].

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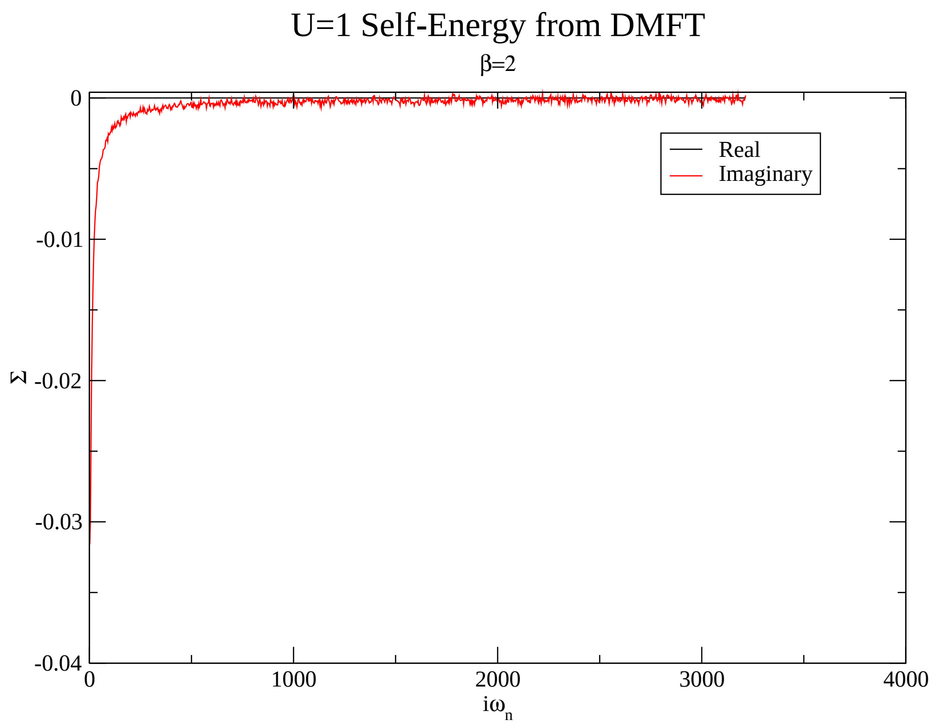
1 Introduction

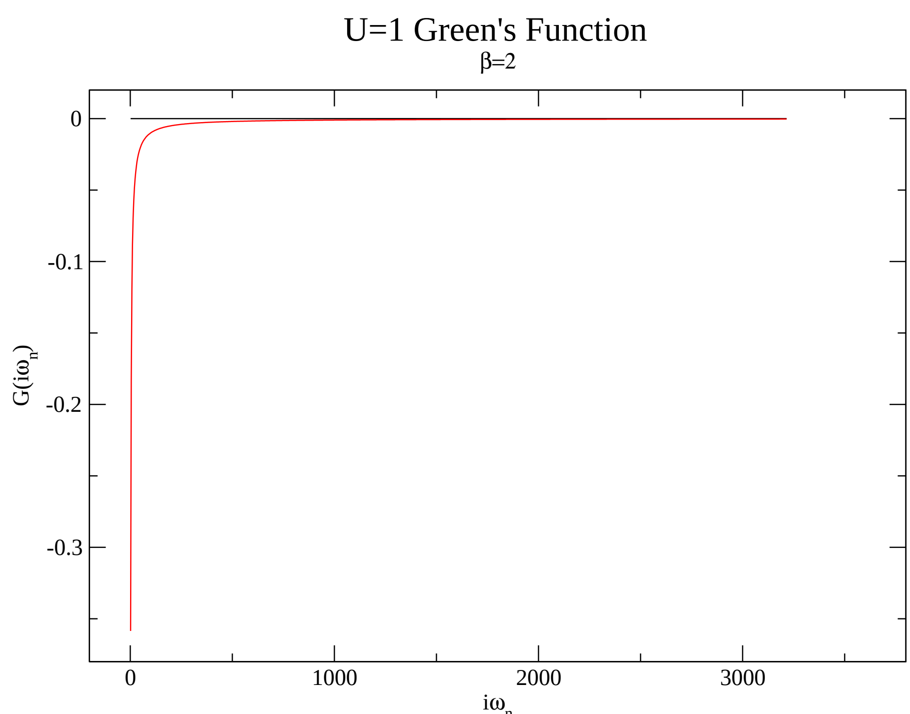
Using DMFT we can set $U = 1$ for a single site at half-filling to generate the interacting Hubbard model

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

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 $A(\omega) = \text{Im}[\Sigma(\omega)]$ 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 $U = 1$, there is a normalization of 0.25.

1.2 Errors

In this case, DMFT self-energies are lacking error bars. Because errors go like $\frac{1}{\sqrt{N}}$ where N is the number of samples, we can instead use this as an order of magnitude estimate for the error. This data had 4296900 sample iterations, and we therefore choose an estimated error $\sigma = 0.0005$.

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: $i\omega_n$ $\mathrm{Re}[\Sigma(i\omega_n)]$ $\mathrm{Im}[G(i\omega_n)]$

  Input file - Selfenergy

  ```
  1.5707963267949 5.6703744085571e-16 -0.03158953764285
  4.7123889803847 3.1444695800992e-16 -0.029847318775471
  7.8539816339745 9.4394785839476e-16 -0.023814398782168
  ```

- *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 -0.03158953764285 0.0005
  4.7123889803847 -0.029847318775471 0.0005
  7.8539816339745 -0.023814398782168 0.0005
  ```

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

  Input file - G_im

  ```
  1.5707963267949 -0.3585154015692 0.0005
  4.7123889803847 -0.18353508163336 0.0005
  7.8539816339745 -0.11976613812711 0.0005
  ```

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

  Input file - G_re

  ```
  1.5707963267949 -2.0386388974517e-17 0.0005
  4.7123889803847 -4.6688456052657e-18 0.0005
  7.8539816339745 -3.4351421175898e-18 0.0005
  ```

3 Using Maxent

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

Param File in.param

```
BETA=2                      #inverse temperature
OMEGA_MAX=25                #the spectral function is wider than omega=10
NDAT=1024                   #num of data points
NFREQ=1000                  #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=0.25                   #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!: 2.30495 Check norm?
Kernel is set up
# 0     4108.32
# 1     1668.62
# 2     513.561
# 3     126.175
# 4     25.6169
# 5     4.3795
# 6     0.635099
# 7     0.0784661
minimal chi2: 0.098459
WARNING: Redefinition of parameter NORM: Input (and output) data are assumed to be
    normalized to NORM.
alpha it: 0     Q = 0.5chi^2-\alpha*entropy: 527.241    norm: 1.16962
alpha it: 1     Q = 0.5chi^2-\alpha*entropy: 481.411    norm: 1.17798
alpha it: 2     Q = 0.5chi^2-\alpha*entropy: 443.307    norm: 1.18585
alpha it: 3     Q = 0.5chi^2-\alpha*entropy: 409.139    norm: 1.19303
alpha it: 4     Q = 0.5chi^2-\alpha*entropy: 378.828    norm: 1.19943
alpha it: 5     Q = 0.5chi^2-\alpha*entropy: 352.116    norm: 1.20499
alpha it: 6     Q = 0.5chi^2-\alpha*entropy: 328.667    norm: 1.2097
alpha it: 7     Q = 0.5chi^2-\alpha*entropy: 308.1      norm: 1.21353
alpha it: 8     Q = 0.5chi^2-\alpha*entropy: 290.018    norm: 1.21649
alpha it: 9     Q = 0.5chi^2-\alpha*entropy: 274.026    norm: 1.21858
alpha it: 10    Q = 0.5chi^2-\alpha*entropy: 259.754    norm: 1.21982
alpha it: 11    Q = 0.5chi^2-\alpha*entropy: 246.864    norm: 1.22024
alpha it: 12    Q = 0.5chi^2-\alpha*entropy: 235.057    norm: 1.21985
alpha it: 13    Q = 0.5chi^2-\alpha*entropy: 224.078    norm: 1.21869
alpha it: 14    Q = 0.5chi^2-\alpha*entropy: 213.717    norm: 1.21679
alpha it: 15    Q = 0.5chi^2-\alpha*entropy: 203.807    norm: 1.21418
alpha it: 16    Q = 0.5chi^2-\alpha*entropy: 194.22     norm: 1.2109
alpha it: 17    Q = 0.5chi^2-\alpha*entropy: 184.869    norm: 1.20697
alpha it: 18    Q = 0.5chi^2-\alpha*entropy: 175.7      norm: 1.20245
alpha it: 19    Q = 0.5chi^2-\alpha*entropy: 166.688    norm: 1.19737
alpha it: 20    Q = 0.5chi^2-\alpha*entropy: 157.834    norm: 1.19178
alpha it: 21    Q = 0.5chi^2-\alpha*entropy: 149.256    norm: 1.18533
alpha it: 22    Q = 0.5chi^2-\alpha*entropy: 140.793    norm: 1.17884
```

```
alpha it: 23    Q = 0.5chi^2-\alpha*entropy: 132.591    norm: 1.17201
alpha it: 24    Q = 0.5chi^2-\alpha*entropy: 124.7      norm: 1.1649
alpha it: 25    Q = 0.5chi^2-\alpha*entropy: 117.171    norm: 1.15758
alpha it: 26    Q = 0.5chi^2-\alpha*entropy: 110.049    norm: 1.15012
alpha it: 27    Q = 0.5chi^2-\alpha*entropy: 103.374    norm: 1.14258
alpha it: 28    Q = 0.5chi^2-\alpha*entropy: 97.1752    norm: 1.13502
alpha it: 29    Q = 0.5chi^2-\alpha*entropy: 91.4723    norm: 1.1275
alpha it: 30    Q = 0.5chi^2-\alpha*entropy: 86.2731    norm: 1.12008
alpha it: 31    Q = 0.5chi^2-\alpha*entropy: 81.5754    norm: 1.11281
alpha it: 32    Q = 0.5chi^2-\alpha*entropy: 77.3674    norm: 1.10573
alpha it: 33    Q = 0.5chi^2-\alpha*entropy: 73.6294    norm: 1.09887
alpha it: 34    Q = 0.5chi^2-\alpha*entropy: 70.3353    norm: 1.09227
alpha it: 35    Q = 0.5chi^2-\alpha*entropy: 67.4542    norm: 1.08595
alpha it: 36    Q = 0.5chi^2-\alpha*entropy: 64.9523    norm: 1.07993
alpha it: 37    Q = 0.5chi^2-\alpha*entropy: 62.7942    norm: 1.07421
alpha it: 38    Q = 0.5chi^2-\alpha*entropy: 60.944     norm: 1.0688
alpha it: 39    Q = 0.5chi^2-\alpha*entropy: 59.3668    norm: 1.0637
alpha it: 40    Q = 0.5chi^2-\alpha*entropy: 58.029     norm: 1.05891
alpha it: 41    Q = 0.5chi^2-\alpha*entropy: 56.8992    norm: 1.05441
alpha it: 42    Q = 0.5chi^2-\alpha*entropy: 55.9485    norm: 1.05021
alpha it: 43    Q = 0.5chi^2-\alpha*entropy: 55.1507    norm: 1.04629
alpha it: 44    Q = 0.5chi^2-\alpha*entropy: 54.4826    norm: 1.04263
alpha it: 45    Q = 0.5chi^2-\alpha*entropy: 53.9235    norm: 1.03923
alpha it: 46    Q = 0.5chi^2-\alpha*entropy: 53.4556    norm: 1.03606
alpha it: 47    Q = 0.5chi^2-\alpha*entropy: 53.0636    norm: 1.0331
alpha it: 48    Q = 0.5chi^2-\alpha*entropy: 52.7344    norm: 1.03035
alpha it: 49    Q = 0.5chi^2-\alpha*entropy: 52.457     norm: 1.02779
alpha it: 50    Q = 0.5chi^2-\alpha*entropy: 52.2225    norm: 1.02541
alpha it: 51    Q = 0.5chi^2-\alpha*entropy: 52.0232    norm: 1.02319
alpha it: 52    Q = 0.5chi^2-\alpha*entropy: 51.8531    norm: 1.02112
alpha it: 53    Q = 0.5chi^2-\alpha*entropy: 51.7072    norm: 1.01919
alpha it: 54    Q = 0.5chi^2-\alpha*entropy: 51.5814    norm: 1.01739
alpha it: 55    Q = 0.5chi^2-\alpha*entropy: 51.4727    norm: 1.01571
alpha it: 56    Q = 0.5chi^2-\alpha*entropy: 51.3782    norm: 1.01415
alpha it: 57    Q = 0.5chi^2-\alpha*entropy: 51.2961    norm: 1.01269
alpha it: 58    Q = 0.5chi^2-\alpha*entropy: 51.2245    norm: 1.01133
alpha it: 59    Q = 0.5chi^2-\alpha*entropy: 51.162     norm: 1.01006
Ng: 5.10747
chi2 max: 105.411
posterior probability of the default model: 1.33065e-33
```

3.1 Output Guide

```
Using flat default model
using kernel fermionic in domain frequency with ph symmetry
The high frequency limit is not 1!: 2.30495 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. In this case, the last few data points are noisy, leading to an inaccurate high frequency limit warning.

```
# 0 4108.32
# 1 1668.62
# 2 513.561
# 3 126.175
# 4 25.6169
# 5 4.3795
# 6 0.635099
# 7 0.0784661
minimal chi2: 0.098459
```

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: 443.307 norm: 1.18585
alpha it: 3 Q = 0.5chi^2-\alpha*entropy: 409.139 norm: 1.19303
...
```

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

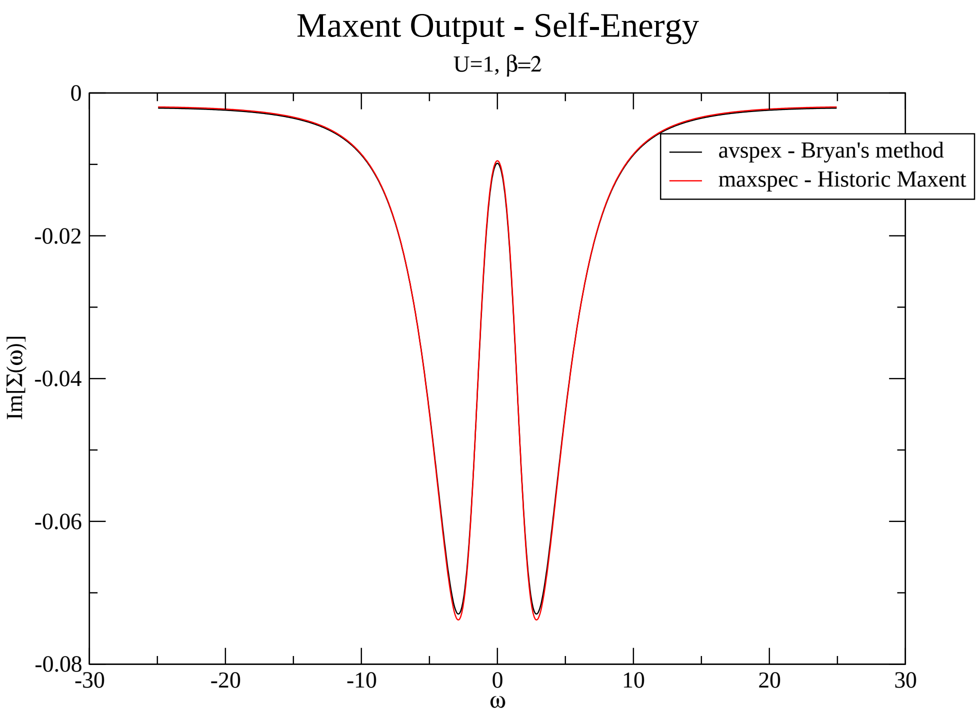
```
Ng: 5.10747
chi2 max: 105.411
posterior probability of the default model: 1.33065e-33
```

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.

If text output is on, Maxent produces 10 files:

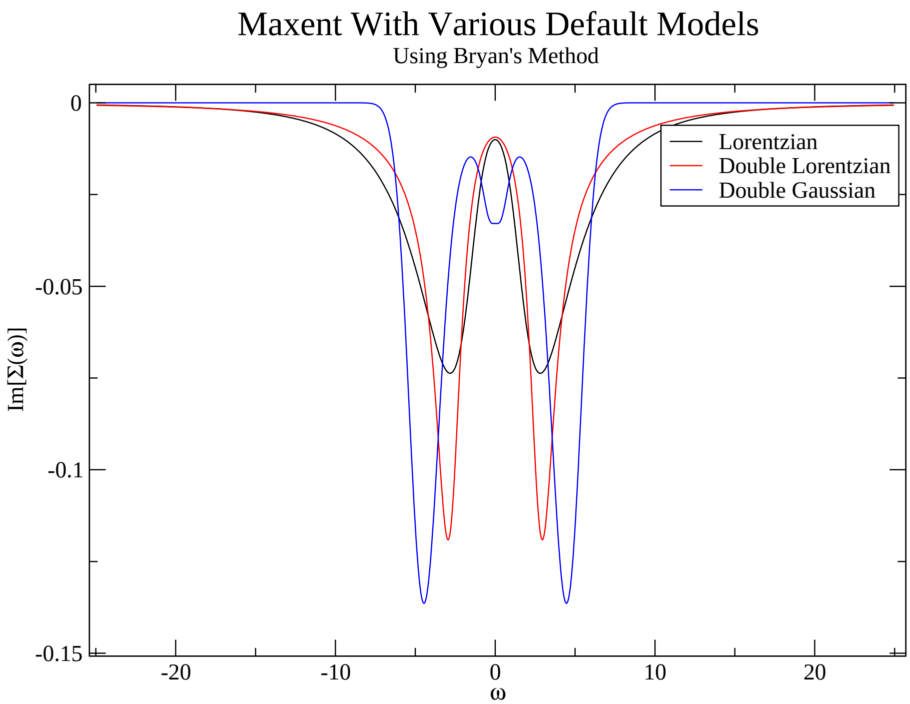
`name.out.avspec.dat`	"Spectral function" using Bayesian Averaging - **Bryan's method**
`name.out.avspec_self.dat`	$\mathrm{Im}[\Sigma(\omega)]$ with the proper sign and normalization; using **Bryan's method**
`name.out.chi2.dat`	Estimated χ^2 for each α value solution
`name.out.chispec.dat`	"Spectral function" satisfying the best χ^2 - **classic Maxent**
`name.out.fits.dat`	Fits of each α value, see comments in file
`name.out.maxspec.dat`	"Spectral function" with the highest probability - **historic Maxent**
`name.out.maxspec_self.dat`	$\mathrm{Im}[\Sigma(\omega)]$ with the proper sign and normalization; using **historic 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 $\sigma = 1, \Gamma = 1, \mu(\text{shift}) = 2.8$. The default model gives a spectral function most similar to a double Lorentzian. When provided with a double Gaussian, Maxent attempts to fit the center peak, but is overcome with the entropy from the Gaussian model underneath.

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`.