Maxent Example - Non-interacting Case

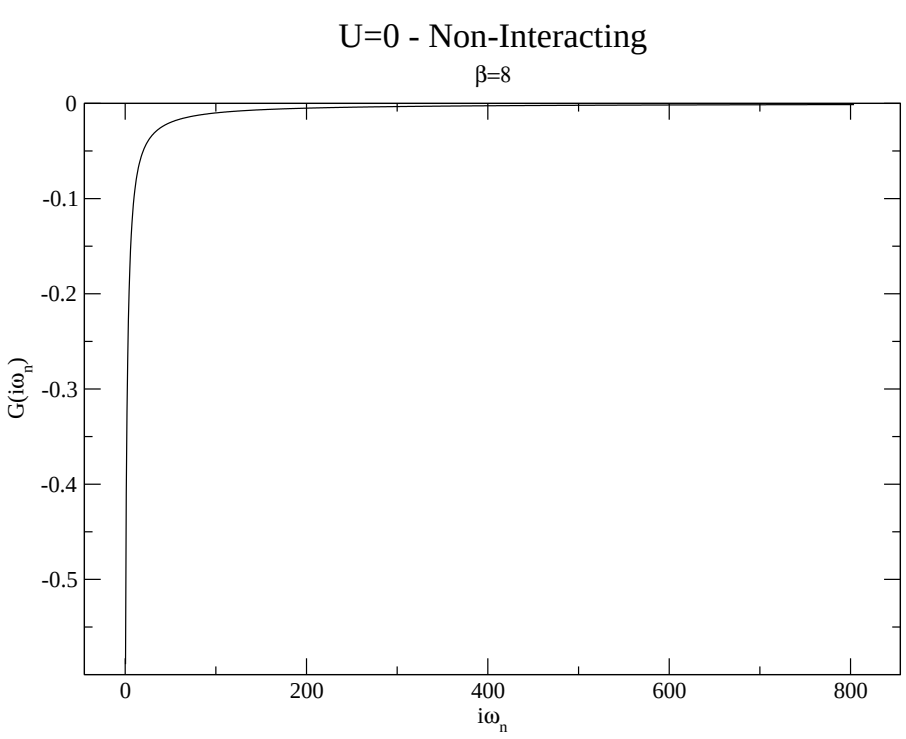
Contents

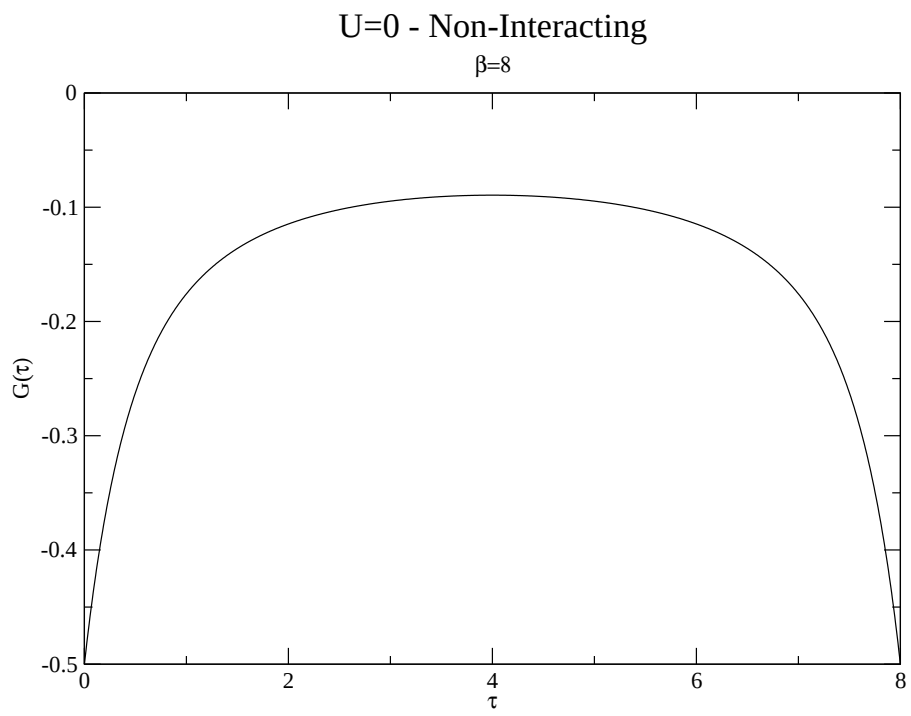
1 Introduction

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

$$H = -t \sum_{<ij>\sigma} c^{\dagger}_{j\sigma} c_{i\sigma}$$

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

2 File Structure

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

Files:

- G_im
  - Im$[G(i\omega_n)]$, 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
```

- Gomegain - $G(i\omega_n)$ input format for maxent
  - index Im$[G(i\omega_n)]$ σ_n

Input file - Gomegain

```
0 -0.58900239090596 1e-05
1 -0.40986302909581 1e-05
2 -0.32440959736089 1e-05
```

- Gtau
  - $G(\tau)$, 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
```

- Gtauin - $G(\tau)$ input format for maxent
  - index $G(\tau)$ σ_τ

Input file - Gtauin

```
0 -0.5 1e-05
1 -0.49377185389756 1e-05
2 -0.48766306852771 1e-05
```

3 Using Maxent

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

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="Gomegain"            #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 $G(\tau)$ is slightly more complex. If your τ grid was created using $\tau_n = n\beta/(ndat-1)$ with n an integer $\in [0, ndat]$, there is no need to supply additional parameters. For any other set of points, you must define `TAU_n =` for each data point.

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 τinput generates a message confirming the choice of τ grid:

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

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 αvalues 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

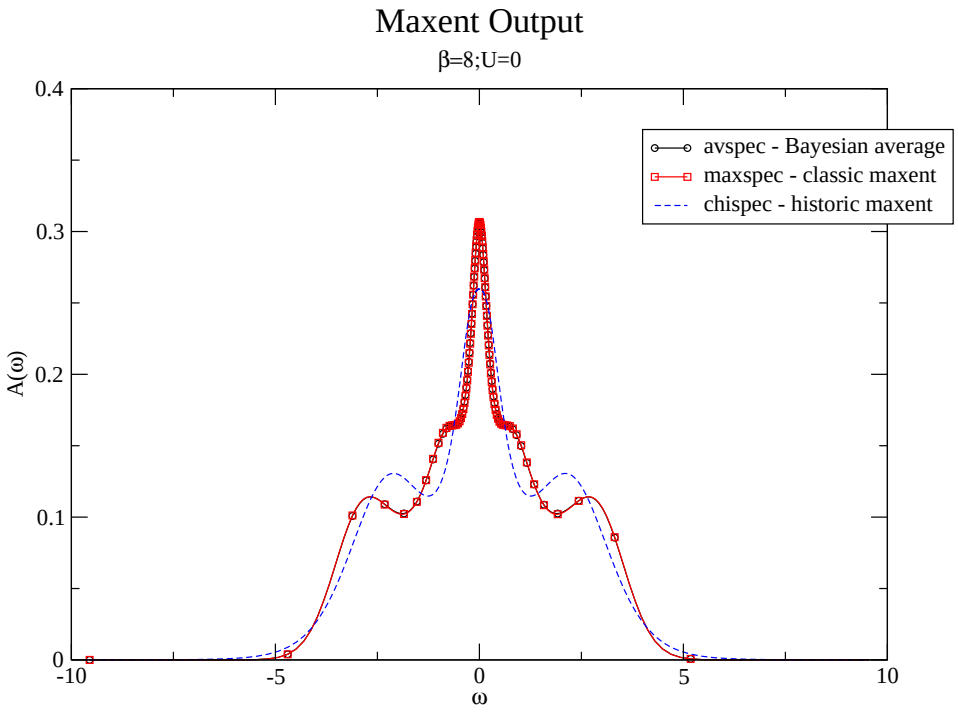
```
Ng: 7.3691
chi2 max: 3.66901
posterior probability of the default model: 1.59791e-24
```

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:

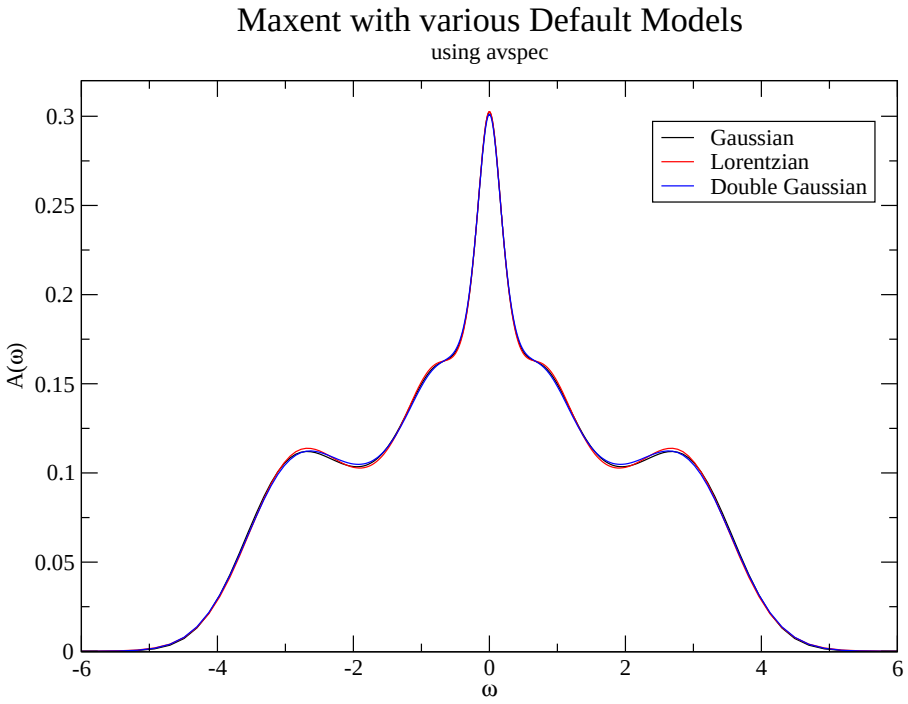
name.out.avspec.dat - Spectral function using Bayesian Averaging
name.out.chi2.dat - estimated χ^2 for each αvalue solution
name.out.chispec.dat - Spectral function satisfying the best χ^2 - **classic Maxent**
name.out.fits.dat - Fits of each αvalue, see comments in file
name.out.maxspec.dat - Spectral function with the highest probability - **historic Maxent**
name.out.out.h5 - all oputput data in the hdf5 format
name.out.prob.dat- the posterior probability of each αvalue
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 $\sigma = 1, \Gamma = 05, \mu(\text{shift}) = 2$. This represents well behaved data within Maxent.