

Maxent Example - Non-interacting Case

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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 (in both τ and $i\omega_n$), and understand the output. This program uses the ALPSCore libraries[\[1, 2\]](#).

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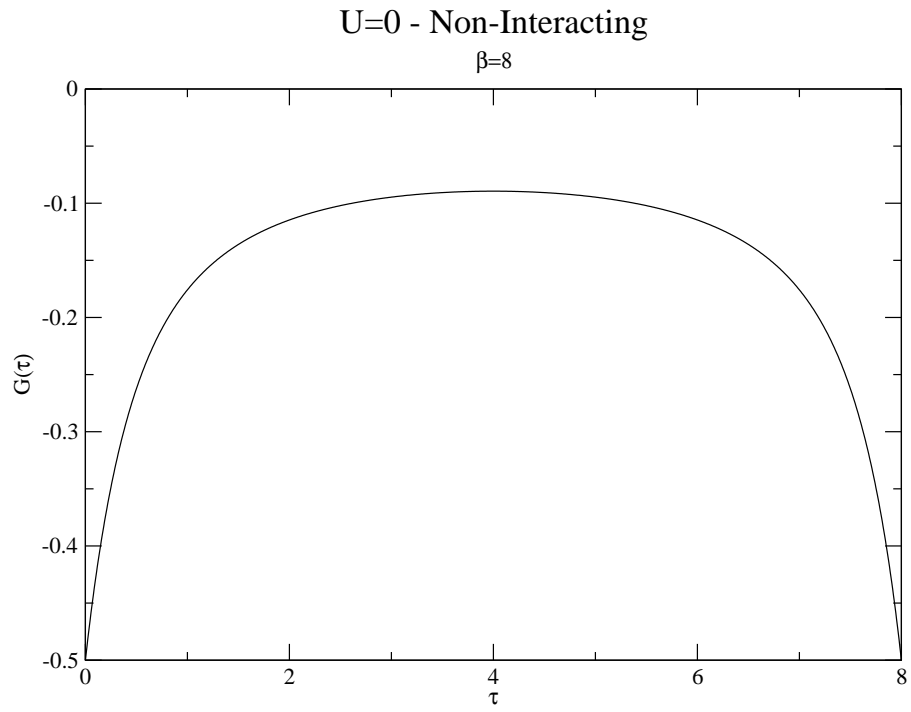
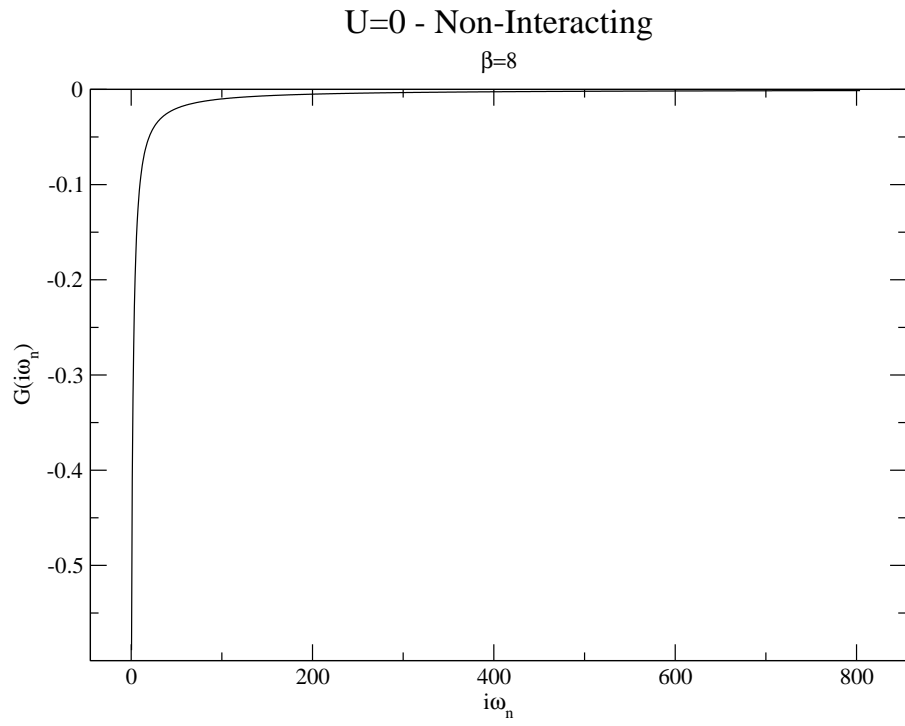
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1 Introduction

Using DMFT we can set $U = 0, \beta = 8$ and generate the non-interacting Hubbard model

$$H = - \sum_{\langle ij \rangle \sigma} t_{ij} \left(c_{i\sigma}^\dagger c_{j\sigma} + c_{j\sigma}^\dagger c_{i\sigma} \right)$$

where $t_{ij} = t = 1$. This produces a Green's function in Matsubara space and Time space:



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	
<ul style="list-style-type: none"> $G_{im} = \text{Im}[G(i\omega_n)]$, also input format for maxent <ul style="list-style-type: none"> column format: $i\omega_n \text{Im}[G(i\omega_n)] \sigma_{I,n}$ 	
Input file - G_im	
<pre>0.39269908169872 -0.58900239090596 1e-05 1.1780972450962 -0.40986302909581 1e-05 1.9634954084936 -0.32440959736089 1e-05</pre>	
<ul style="list-style-type: none"> $G_{re} = \text{Re}[G(i\omega_n)]$ <ul style="list-style-type: none"> column format: $i\omega_n \text{Re}[G(i\omega_n)] \sigma_{R,n}$ 	
Input file - G_re	
<pre>#Freq 0 1e-05 0.39269908169872 4.1987536135299e-16 1e-05 1.1780972450962 2.1665780666625e-16 1e-05</pre>	
<ul style="list-style-type: none"> $G_{\tau} = G(\tau)$, also input format for maxent <ul style="list-style-type: none"> column format: $\tau G(\tau) \sigma_{\tau}$ 	
Input file - Gtau	
<pre>0 -0.5 1e-05 0.0078125 -0.49377185389756 1e-05 0.015625 -0.48766306852771 1e-05</pre>	

3 Using Maxent

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

Param File in.param	
BETA=8	<i>#inverse temperature</i>
NDAT=1024	<i>#num of data points</i>
NFREQ=500	<i>#num of output frequencies</i>
DATASPACE=frequency	<i>#G(iω)</i>
KERNEL=fermionic	<i>#fermionic/bosonic values</i>
PARTICLE_HOLE_SYMMETRY=1	<i>#generated at half-filling; only use imag part</i>
DATA="G_im"	<i>#location of data file</i>

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	4.43997e+06		
# 1	824689		
# 2	183134		
# 3	48665.1		
# 4	12070		
# 5	2651.32		
# 6	515.856		
# 7	88.4136		
minimal chi2: 2.5094e-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: 988044 norm: 1.03401			
alpha it: 1 WARNING: iteration reached max_it without converging, your minimizer is having problems. Please be careful!			
Q = 0.5chi^2-\alpha*entropy: 155.177 norm: 1.00046			
alpha it: 2	Q = 0.5chi^2-\alpha*entropy: 93.4638	norm: 1.00035	
alpha it: 3	Q = 0.5chi^2-\alpha*entropy: 82.0855	norm: 1.00033	
alpha it: 4	Q = 0.5chi^2-\alpha*entropy: 72.0537	norm: 1.0003	
....	
alpha it: 55	Q = 0.5chi^2-\alpha*entropy: 0.0395432	norm: 1.00001	
alpha it: 56	Q = 0.5chi^2-\alpha*entropy: 0.0337686	norm: 1.00001	
alpha it: 57	Q = 0.5chi^2-\alpha*entropy: 0.0287851	norm: 1	
alpha it: 58	Q = 0.5chi^2-\alpha*entropy: 0.0245047	norm: 1	
alpha it: 59	Q = 0.5chi^2-\alpha*entropy: 0.0208447	norm: 1	
Ng: 7.36894			
posterior probability of the default model: 1.59874e-24			
spectra	max backcont diff	chi^2 value	
=====	=====	=====	
chispec	0.000488947	278.701	
avspec	0.000428287	4.38837	
maxspec	0.00042735	3.6677	

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 #generated at half-filling
DATASPACE=time  #G( $\tau$ )
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 4.43997e+06
# 1 824689
# 2 183134
# 3 48665.1
# 4 12070
# 5 2651.32
# 6 515.856
# 7 88.4136
minimal chi2: 2.5094e-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: 93.4638 norm: 1.00035
alpha it: 3 Q = 0.5chi^2-\alpha*entropy: 82.0855 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 ≈ 1 for all iterations

Ng: 7.36894 posterior probability of the default model: 1.59874e-24
--

This is posted after completing all α values and root finding. Ng represents the number of “good input points,” 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.

spectra	max backcont diff	chi^2 value
=====	=====	=====
chispec	0.000488947	278.701
avspec	0.000428287	4.38837
maxspec	0.00042735	3.6677

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.

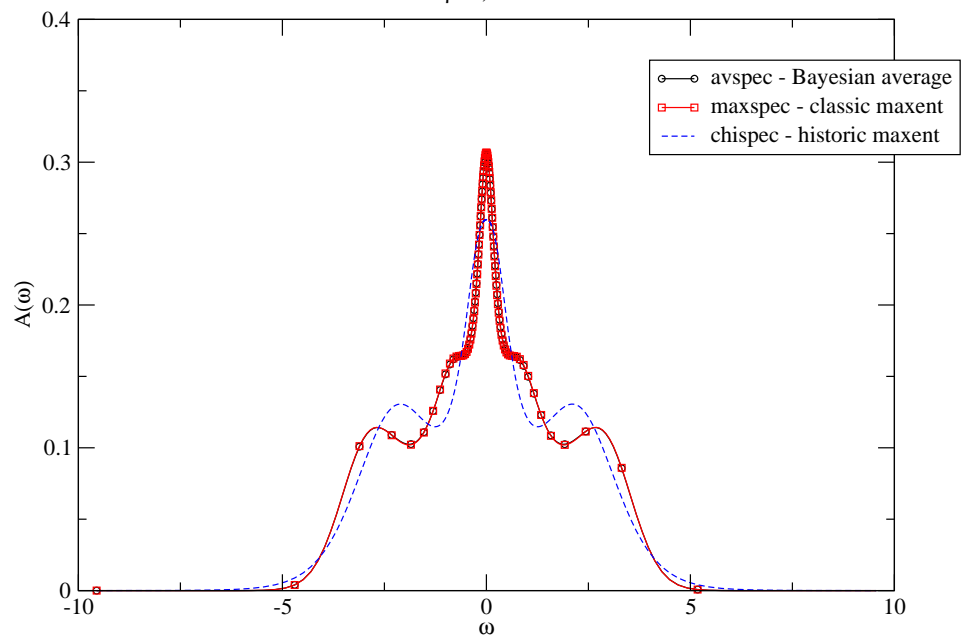
If text output is on, Maxent produces 11 files:

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.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.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:

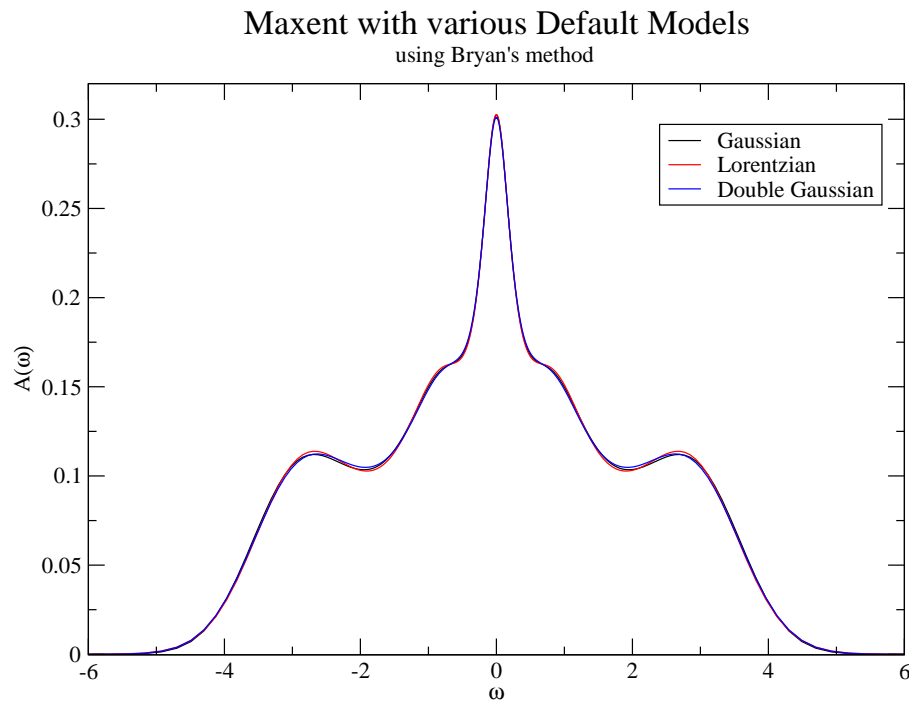
Maxent Output

$\beta=8; U=0$



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, 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](https://doi.org/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](https://doi.org/10.1088/1742-5468/2011/05/P05001).