Maxent Example - Legendre Basis

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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 a Green's function expanded using Legendre polynomials, and understand the output. This program uses the ALPSCore libraries[1, 2].

Contents

1 Introduction

Using an arbitrary spectral function, we can use a technique developed by Boehnke, et al[3] to determine the corresponding Green's function in the Legendre basis. This basis can be characterized by the relationship to the spectral function as

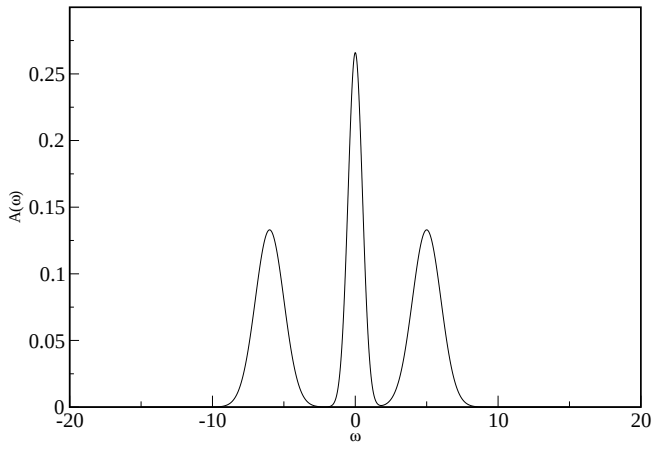
$$\begin{aligned} G_\ell &= \int_{-\infty}^{\infty} d\omega A(\omega) K(\ell, \omega) \\ &= -\int_{-\infty}^{\infty} d\omega A(\omega) \int_0^\beta d\tau \sqrt{2\ell+1} \frac{e^{-\tau\omega}}{1+e^{-\beta\omega}} P_\ell(x(\tau)), \end{aligned}$$

where $P_\ell(t)$ is the ℓth Legendre polynomial and $x(\tau) = 2\tau/\beta - 1 \in [-1, 1]$.

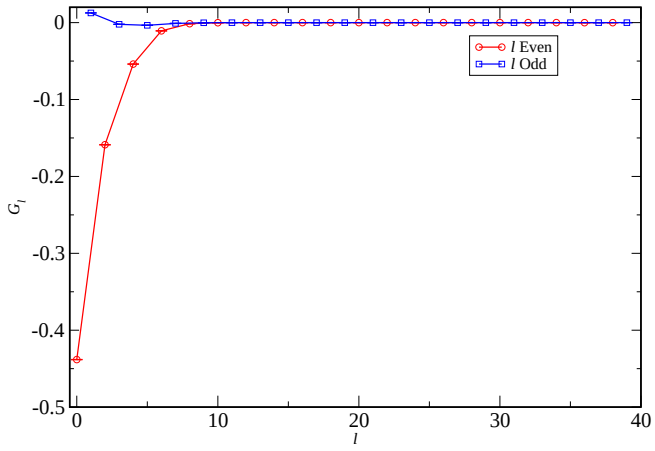
In this example, we'll use the spectral function and G_ℓ shown in Figure 1.

2 File Structure

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



(a) Spectral function



(b) Corresponding Legendre basis representation

Figure 1: Data for this example

Filenames and Descriptions

- *Spect_in* = $A(\omega)$
  - column format: ω $A(\omega)$

Input file - Spect_in

```
-15.0 3.4265911905563055e-19
-14.9899966656 3.7492128889364698e-19
-14.9799933311 4.10179971231302e-19
```

- *Gl.dat* = G_ℓ, also input data format for maxent
  - column format: ℓ G_ℓ σ_ℓ

Input file - Gl.dat

```
0 -0.43821467393467 2.0578273007296e-08
1 0.012631583637553 2.0389308663417e-08
2 -0.15880101626593 2.1475723695007e-08
```

3 Using Maxent

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

Param File in.param

```
BETA = 2                        #inverse temperature
NDAT = 10                       #num of data points
DATASPACE=Legendre              #G(ℓ)
KERNEL=fermionic                #fermionic values
DATA=gl.dat                     #location of data file
PARTICLE_HOLE_SYMMETRY=1        #This example has PH symmetry
NFREQ=5000                      #increase omega grid for better
```

```
                          #integration and convergence
FREQUENCY_GRID=quadratic  #use more points away from origin
N_ALPHA=15                #reduce number alpha search space
```

Maxent then produces the following output:

Maxent output

```
Using flat default model
using kernel fermionic in domain legendre with ph symmetry
Kernel is set up
# 0     1.80993e+09
# 1     1.16275e+09
# 2     5.32206e+08
# 3     2.48624e+08
# 4     1.02973e+08
# 5     3.80307e+07
# 6     1.27156e+07
# 7     3.69596e+06
# 8     999676
# 9     250449
minimal chi2: 5.99347e-18
alpha it: 0     WARNING: iteration reached max_it without converging, your
    minimizer is having problems. Please be careful!
Q = 0.5chi^2-\alpha*entropy: 1.3593e+10 norm: 1.01217
alpha it: 1     WARNING: iteration reached max_it without converging, your
    minimizer is having problems. Please be careful!
Q = 0.5chi^2-\alpha*entropy: 882002     norm: 1.00004
alpha it: 2     Q = 0.5chi^2-\alpha*entropy: 4.78239    norm: 0.999915
...
alpha it: 14    WARNING: iteration reached max_it without converging, your
    minimizer is having problems. Please be careful!
Q = 0.5chi^2-\alpha*entropy: 0.00708256 norm: 0.999915
Ng: 138.545
posterior probability of the default model: 2.97843e-43
spectra     max backcont diff    chi^2 value
=======     =================    ===========
chispec        7.50655e-08       4.23956e-06
avspec         7.50659e-08       1.54179e-11
maxspec        7.50659e-08       1.54179e-11
```

3.1 Output Guide

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

These are the setup messages, confirming your input choices.

```
# 0 1.80993e+09
# 1 1.16275e+09
# 2 5.32206e+08
# 3 2.48624e+08
# 4 1.02973e+08
# 5 3.80307e+07
# 6 1.27156e+07
# 7 3.69596e+06
# 8 999676
# 9 250449
minimal chi2: 5.99347e-18
```

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: 0 WARNING: iteration reached max_it without converging,
your minimizer is having problems. Please be careful!
Q = 0.5chi^2-\alpha*entropy: 1.3593e+10 norm: 1.01217
alpha it: 1 WARNING: iteration reached max_it without converging,
your minimizer is having problems. Please be careful!
Q = 0.5chi^2-\alpha*entropy: 882002 norm: 1.00004
alpha it: 2
Q = 0.5chi^2-\alpha*entropy: 4.78239 norm: 0.999915
...
```

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. Because the Legendre kernel is so small, some of the last α values will struggle to converge. Notice that the norm stays $\approx$1 for all iterations

```
Ng: 138.545
posterior probability of the default model: 2.97843e-43
```

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.

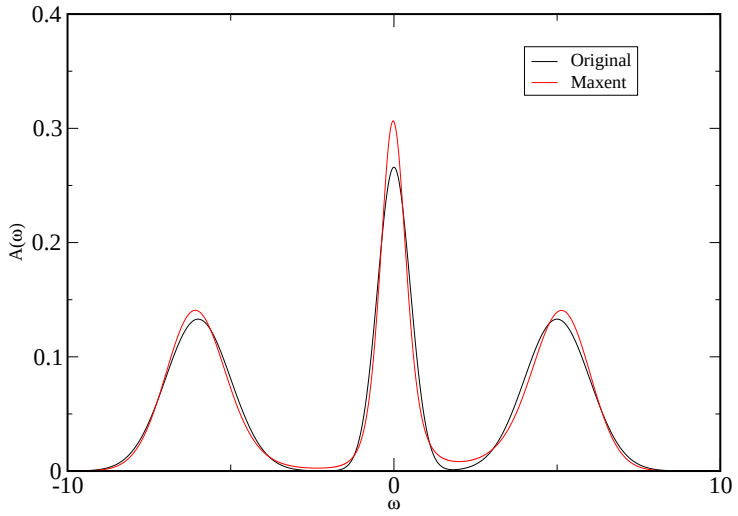
```
spectra     max backcont diff    chi^2 value
=======     =================    ===========
chispec        7.50655e-08       4.23956e-06
avspec         7.50659e-08       1.54179e-11
maxspec        7.50659e-08       1.54179e-11
```

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.

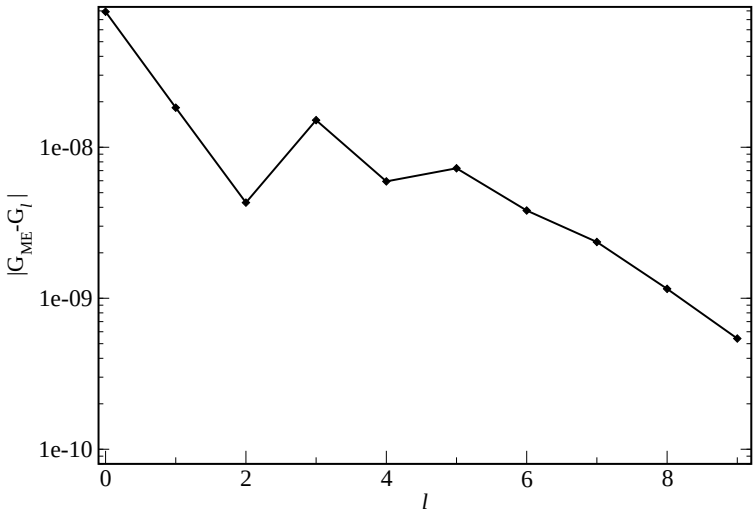
If text output is on, Maxent produces 11 files:

`name.out.avspec.dat`	Spectral function using Bayesian Averaging - **Bryan's method**
`name.out.avspec_back.dat`	The `avspec` spectrum continued back to the Legendre basis
`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 Legendre basis
`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 Legendre basis
`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:



where the error on the imaginary axis is



With this the maxent procedure can be considered successful, because the error on the back-continuation is on the order of the input error bars.

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.

[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.

[3] Lewin Boehnke, Hartmut Hafermann, Michel Ferrero, Frank Lechermann, and Olivier Parcollet. Orthogonal polynomial representation of imaginary-time green's functions. *Phys. Rev. B*, 84:075145, Aug 2011. URL: http://link.aps.org/doi/10.1103/PhysRevB.84.075145, doi:10.1103/PhysRevB.84.075145.