Maxent - Advanced Feature Guide

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Abstract

This document is a tutorial on the advanced features of Maxent, a program for performing analytical continuation using the maximum entropy method. It will explain how to use a custom default model, the model runs feature, and error calculation. This program uses the ALPSCore libraries[1, 2].

Contents

1 Custom Default Model **1**

2 Model Runs **1**

3 Error Calculation **2**
3.1 Theory 2
3.2 User Guide 2

References **3**

1 Custom Default Model

To use a custom default model, simply create a file with the default model in the format

```
...
omega_n D(omega_n)
omega_n+1 D(omega_n+1)
...
```

Then for the default model parameter, use the filename as the parameter, (e.g. for the file "def.dat" the parameter would be `DEFAULT_MODEL=''def.dat''`). The default model must be within the correct bounds of your parameter file as well as be normalized; some checks for errors like these are also performed in the code.

2 Model Runs

To perform multiple Maxent calculations using different default models, one can use the `--MODEL_RUNS` command. For example, for 3 different default model choices (flat, Gaussian, Lorentzian), the following would be required in the param file

```
MODEL_RUNS=3
RUN_0 = "flat"
RUN_1 = "Gaussian"
RUN_2 = "Lorentzian"
#Default model settings
SIGMA=1
GAMMA=0.5
```

This will produce files `name.out.(Default model).___.dat` if text_output is on. Note that there is no way to currently vary the default model parameters within these runs; this feature must be scripted externally.

After running the default models, a new file will be generated `name.out.varspec.dat`. The first line of the file explains the output

```
#omega mean_maxspec stdev_maxspec mean_avspec stdev_avspec
-9.180009739 2.193129306e-11 3.101553208e-11 9.76310756e-11 1.380711912e-10
-7.77085514 5.465279583e-09 7.729072509e-09 1.180425604e-08 1.669373898e-08
....
```

The first column is the ω value of the spectral function, the second/third and fourth/fifth are the mean/standard deviation of the maxspec and avspec output respectively.

3 Error Calculation

3.1 Theory

Jarrell and Gubernatis in their analysis of the maximum entropy method[3], defined for a given most probable α and corresponding A_α, the positive-definite matrix $\Gamma_{ij} = \alpha\delta_{ij} + \Lambda_{ij}$ where

$$\begin{aligned}\Lambda_{ij} &= \sqrt{A_i}\frac{\partial^2 L}{\partial A_i \partial A_j}\sqrt{A_j}\Big|_{A=A_\alpha} \\ &= \sqrt{A_i}[K^T C^{-1} K]_{ij}\sqrt{A_j}\Big|_{A=A_\alpha}\end{aligned}$$

where C is the covariance matrix on the input data and K the kernel. After moving into a convenient basis where the curvature of the entropy is constant and moving back, one can write that the covariance X of the spectral function output is given as

$$X_{ij} = \langle \delta A_i \delta A_j \rangle \approx \sqrt{A_i}\,[\Gamma^{-1}]_{ij}\sqrt{A_j}.$$

Note that this is only a second order approximation to the covariance matrix, and thus will fail for certain datasets.

In order to use the bootstrap routine to determine the error from the covariance matrix, the covariance must be diagonal. Thus we can determine a basis where the covariance is diagonal, bootstrap in this basis, and transform back. The transformation matrices are given by solutions to the eigenvalue problem,

$$\begin{aligned}\Gamma &= U^{-1}DU = U^T DU, \\ \implies \Gamma^{-1} &= UD^{-1}U^T,\end{aligned}$$

where D is a diagonal matrix of eigenvalues and U is a matrix whose columns are eigenvectors of Γ. Because Γ is positive-definite, we can use the fact that U is orthogonal. Thus we have a diagonal covariance X_D which can be written

$$[X_D]_{ij} = \left(\sqrt{A_i}U_{ij}\right) D_{ij}^{-1} \left(U_{ij}^T\sqrt{A_j}\right).$$

We can perform a bootstrap in the diagonal basis, then transform back using U. Note that this is using the metric of $\sqrt{A}$, so after bootstrapping we must square our vector to get out the original A. This overcomes the fact that $\sqrt{A}$ during bootstrap may become negative.

3.2 User Guide

To calculate errors for a particular calculation, use the parameter `GENERATE_ERR` which takes a boolean value; by default this is false. Thus when `GENERATE_ERR=true` is added to a parameter file (or via command line by `-GENERATE_ERR=''true''`), the statement

Finished generating A*u + Gaussian Noise

is added before the back-continuation routine (if enabled), as well as the new file `name.out.booterr.dat`. Inside the file, the first line is a comment describing the columns of data

#omega A A_mean approx_err

To plot the spectral function `maxspec` (the most probable spectral function), one can use the 1st column ω vs the second column $\hat{A}(\omega) = A_{maxspec}(\omega)$ with error bars of the fourth column.

To also get a sense of the off diagonal elements of the covariance matrix, the average spectral function from the bootstrap routine is also included as the third column. This is most helpful plotted against `maxspec`, i.e. both the second and third column.

For certain parameters, the second order approximation to the error will fail, in which maxent will report

Error! Something has gone wrong with the error bars. Please check your settings!

If this appears, the number of frequencies may be too few, the error of the input data may be incorrect, or something more serious like an incorrect `BETA` or `NDAT` value.

References

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

[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] Mark Jarrell and James E Gubernatis. Bayesian inference and the analytic continuation of imaginary-time quantum monte carlo data. *Physics Reports*, 269(3):133–195, 1996.