Stochastic Optimization for Quantum Materials Simulations

OAK RIDGE National Laboratory | CompFUSE Computational Framework for Unbiased Studies of Correlated Electron Systems

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Stochastic Optimization for Analytical Continuation

Background

Quantum Monte Carlo (QMC) methods provide numerically exact results for interacting quantum many-particle systems and thus are widely used to study their physics. The analytic continuation of imaginary-time QMC data to extract real-frequency spectra remains a key problem in connecting theory with experiments. In this work, we present a fast and efficient stochastic optimization method (FESOM) as a more accessible variant of the stochastic optimization method introduced by Mishchenko [Phys, Rev. B 62, 6317 (2000)].
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Analytical Continuation

❖ The analytic continuation process involves an inversion of the integral

$$G(\mathrm{i}w_n) = \int dw\, K(iw_n, w)A(w)$$

- $\mathrm{G}(\mathrm{i}w_n)$ is an observable such as the single-particle Green's function measured in a QMC calculation of discrete Matsubara frequencies w_n
- $A(w)$ is the spectral function and the quantity of interest
- $K(iw_n, w) = \frac{1}{iw_n - w}$ is the kernel

❖ The discretized analytical continuation is given as follows

$$G_n = \sum_{l=1}^{L} K_{nl} A_l$$

- L is the number of partitions in real axis
- $G_n = G(\mathrm{i}w_n)$
- $K_{nl} = \frac{\Delta w_l}{iw_n - w_l}$
- $A_l = A(w)$

➢ The difficulty of analytical continuation arises from the fact that the matrix K_{nl} is ill-conditioned, i.e. small errors in the QMC data G_n cause large errors in the quantity of interest A_l and there are an infinite number of solutions.

FESOM

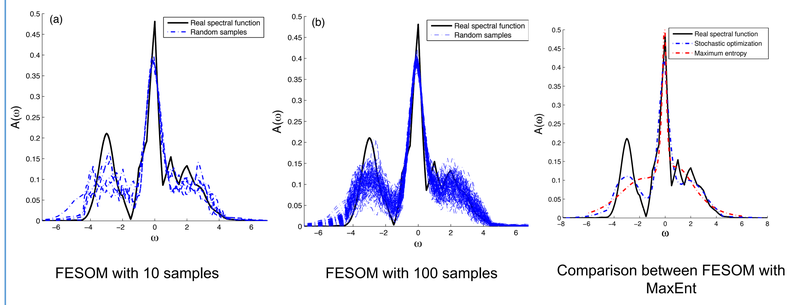
FESOM adopts the Bayesian framework to address the ill-posedness of the kernel matrix. We assume the prior distribution is uniform and focus on estimating spectral function by the mean value of the likelihood. The algorithm is composed by the following procedures:

- Initialize R realizations of the spectral function A with the initial guess D, denoted by $A_0^r(w_l) = D(w_l)$
- For the r-th sample $A_i^r(w_l)$, we add a Gaussian process λ_i^r to get a propose spectral function $A_{i+\frac{1}{2}}^r(w_l)$
- If the proposed spectral function $A_{i+\frac{1}{2}}^r$ fits the data better than the previous A_i^r, we accept the update and set $A_{i+1}^r = A_{i+\frac{1}{2}}^r$. Otherwise, the update is rejected and $A_{i+1}^r = A_i^r$
- Calculate the final estimated spectral function by averaging all the samples, i.e. $\bar{A}(w_l) = \frac{1}{R}\sum_{r=1}^{R} A_i^r(w_l)$

Performance

❖ We demonstrate the performance of FESOM and compare FESOM with Maximum Entropy method (MaxEnt)

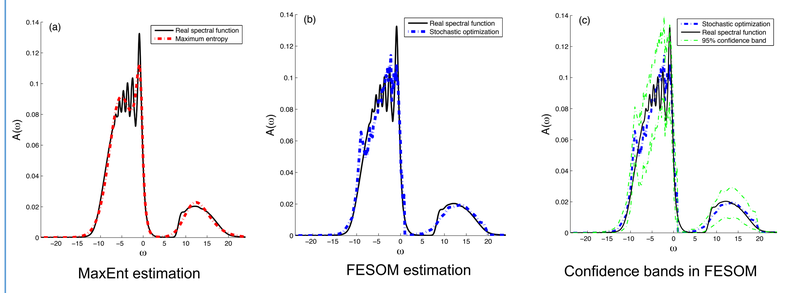
Synthetic spectral function



FESOM with 10 samples | FESOM with 100 samples | Comparison between FESOM with MaxEnt

➢ FESOM estimation is better than the MaxEnt

Two dimensional Hubbard model



MaxEnt estimation | FESOM estimation | Confidence bands in FESOM

➢ Samples in FESOM capture the confidence band for the spectral function

Stochastic Optimization for Dynamic Cluster Approximation

Background

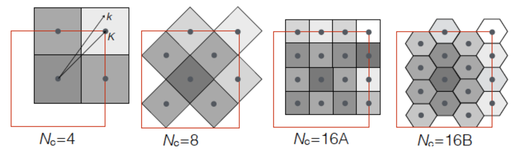
The dynamical cluster approximation (DCA) is a systematic extension beyond the single-site approximation in dynamical mean field theory, to include spatially nonlocal correlations in quantum many-body simulations of strongly correlated systems. The DCA uses coarse-graining of the momentum space to reduce the complexity of quantum many-body problems, thereby mapping the bulk lattice to a cluster embedded in a dynamical mean-field host. The DCA+ [Staar et al., Dynamical Cluster, Phys. Rev. B 88, 115101 (2013).] method extends the DCA through the inclusion of a self-energy with continuous momentum dependence. Here, we present a stochastic optimization method (SOM) that reconstructs the continuous self-energy calculated in the DCA+ from the self-energy calculated on the cluster.

SOM for DCA+

❖ DCA+ extends DCA through the inclusion of a lattice self-energy with continuous momentum dependence which gives the relation

$$\Sigma_c(K, iw_n) = \frac{N_c}{N}\sum_k \phi_K(k)\,\Sigma^{DCA+}(k, iw_n) \qquad (1)$$

- $\Sigma_c(K, iw_n)$ is the cluster self-energy
- $\Sigma^{DCA+}(k, iw_n)$ is the DCA+ lattice self-energy
- $\phi_K(k)$ is the patch function with N_c patches



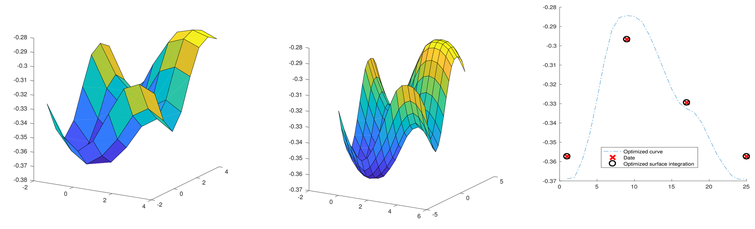
Different patching of the momentum space

❖ The SOM constructs a smooth self-energy surface that satisfies the identity (1).

- The SOM uses the interpolated cluster self-energy as the initial condition to start the algorithm
- At each iteration step, we perturb the previous self-energy surface by a Gaussian process and accept the proposed self-energy surface that satisfies (1) better
- The SOM is implemented on the coarse grids, and then refined on the finer girds

Performance

❖ We use four point cluster data as an example to demonstrate the performance of SOM for DCA+



SOM reconstructed self-energy surface on coarse grids | SOM reconstructed self-energy surface on fine grids | Fitting of SOM to the original cluster data

Table: Error comparison

Type of approximation	Error
DCA+ continuous surface	0.0256
$\mathrm{SOM}_{\mathrm{Coarse\ mesh}}$	1.1339×10^{-5}
$\mathrm{SOM}_{\mathrm{Coarse\ mesh\ interpolated}}$	6.3038×10^{-4}
$\mathrm{SOM}_{\mathrm{Fine\ mesh}}$	2.8465×10^{-5}

➢ SOM constructs smooth self-energy and fits the cluster data

Summary

- Stochastic optimization could address difficulties encountered by deterministic methods
- It gives rigorous estimation for the quantity of interests in quantum materials simulations
- The scalability of stochastic optimization makes the algorithm flexible and is especially suitable for high performance computing facilities

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