Analytic Continuation of Noisy Data Using Multistep Neural Network

Oak Ridge National Laboratory | Center for Nanophase Materials Sciences

Xuping Xie, Feng Bao, Thomas Maier and Clayton Webster

xiex@ornl.gov, fbao@fsu.edu, maierta@ornl.gov, webstercg@orn.gov

Oak Ridge National Laboratory

Contribution: A new Data-Driven framework

We propose a new data-driven framework for analytic continuation problem using deep neural network architecture. A novel *linear multistep network architecture* is used for learning the kernel in the inversion process.

Analytic Continuation

The imaginary time Matsubara Green's functions $G(\tau)$, which are the fundamental objects that most QMC method produce as a simulation output,

$$\begin{aligned} G(\tau) &= \int KA(\omega)d\omega \\ K &= \frac{e^{-\omega\tau}}{1+e^{-\omega\beta}} \end{aligned} \tag{1}$$

where K is the Kernel of the analytic continuation, $A(\omega)$ is the spectral function defined on real axis. Calculations is often tractable in the imaginary time domain. The challenge is to obtain a spectral function from imaginary Green's function. The continuation process is an ill-posed problem, and the direct inverse $A = K^{-1}G$ is hardly feasible due to the high condition number.

Maximum Entrophy (MaxEnt)

The least square fitting is applied to M samples of $G^i(\tau)$,

$$\min \frac{1}{2}\chi^2 - \alpha S[A] \tag{5}$$

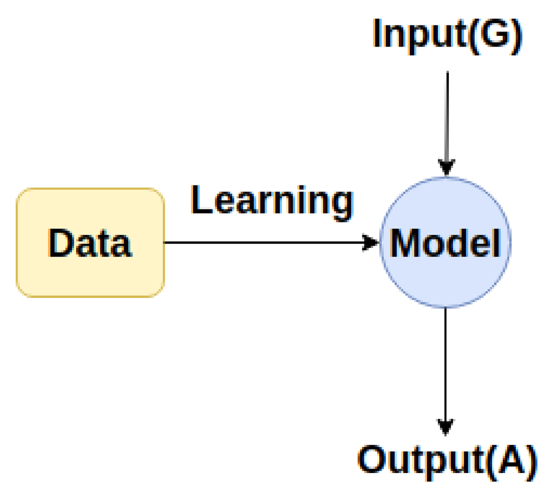
$$\chi^2 = \sum_{n,m}^{M}(G^i(\tau_m) - G(\tau_n))^2\sqrt{C_{nm}} \tag{6}$$

where C_{mn} being the covariance matrix, $S = -\int A(\omega)\ln[\frac{A(\omega)}{\bar{A}(\omega)}]d\omega$ is the entropy term that regularize the problem. If the input data is uncorrelated then only the diagonal elements of the covariance matrix are non-zero, in which case χ^2 takes the form

$$\chi^2 = \sum_{n}^{M}\frac{(\overline{G}(\tau_m) - G(\tau_n))^2}{\sigma^2}$$

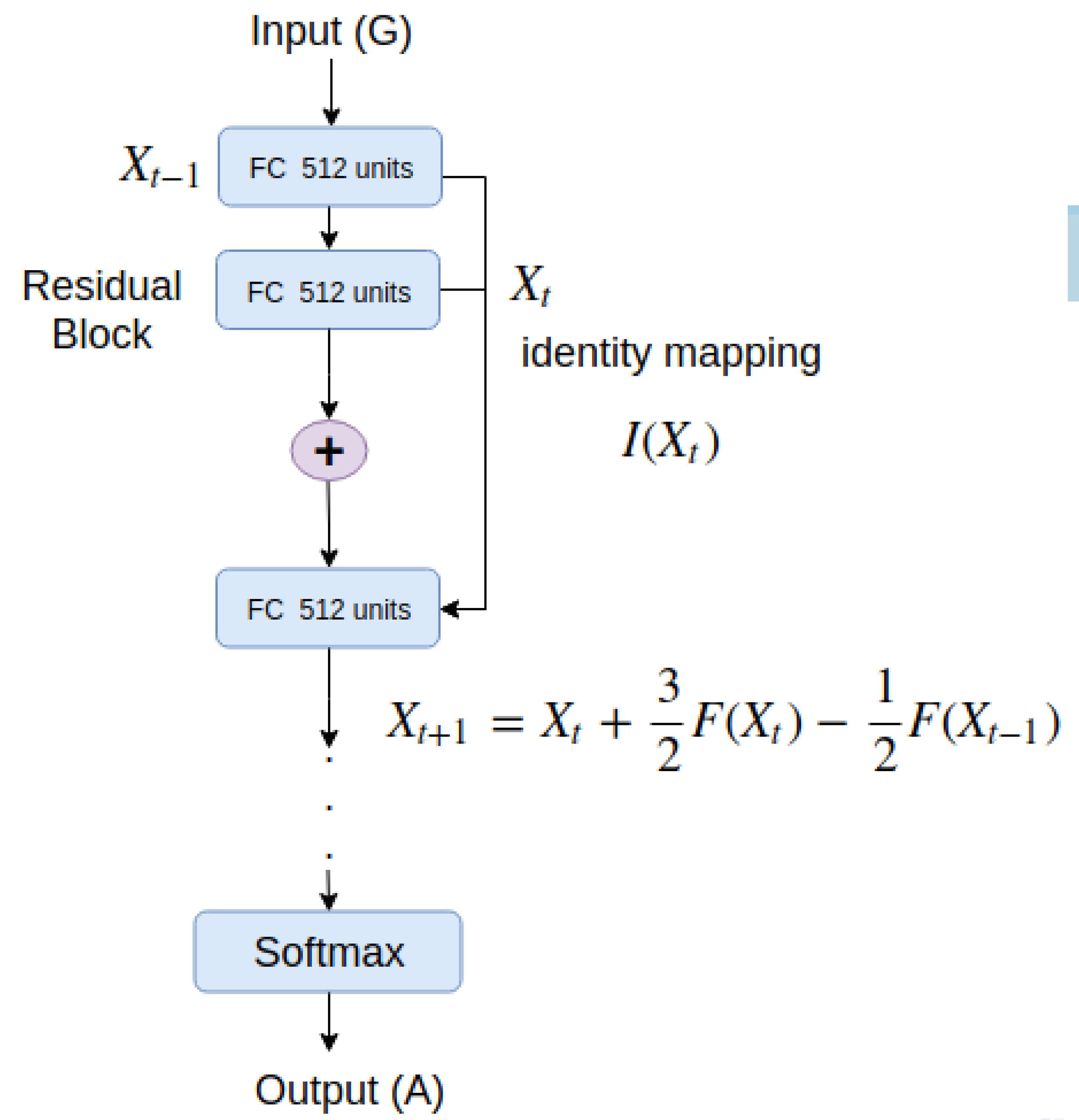
Data-Driven Learning

The following is the general learning framework,



Mulistep Residual Neural Nets

This idea coming from image processing, inverse problem field,



References

[1] Xie, X., Bao, F., Maier, T. and Webster, C., 2019. Analytic Continuation of Noisy Data Using Adams Bashforth ResNet. arXiv preprint arXiv:1905.10430.

Mathematicla Formulation

We stack the training features and target row-wise into matrices $\boldsymbol{X}_0 = [G^1, G^2, ..., G^s]^T \in R^{s\times n}$ and $\boldsymbol{A} = [A^1, A^2, ..., A^s] \in R^{s\in N}$. The forward propagation of the network can be considered as the forward Euler discretization of the initial value ODE

$$\dot{\boldsymbol{X}}(t) = \sigma(\boldsymbol{X}(t), \boldsymbol{W}(t), b(t)), \;\; \boldsymbol{X}(0) = \boldsymbol{X}_0, \;\; 0 \le t \le T \tag{2}$$

where time t corresponds to the direction from input to output, $\boldsymbol{X}(0)$ is the initial input feature, and $\boldsymbol{X}(T)$ is the output of the network. We use two step Adams-Bashforth (AB) method to discretize the neural network, the architecture can be found at Fig. This learning process can be solved by the following optimization problem

$$\min L(\tilde{\boldsymbol{A}}, \boldsymbol{A}) + \lambda R(\boldsymbol{W}, b) \tag{3}$$

The loss function $L(\tilde{\boldsymbol{A}}, \boldsymbol{A}) = 1/2\|\tilde{\boldsymbol{A}} - \boldsymbol{A}\|_F^2$ is the sum of squared difference. L^2 regularizer R is applied to prevent overfitting.

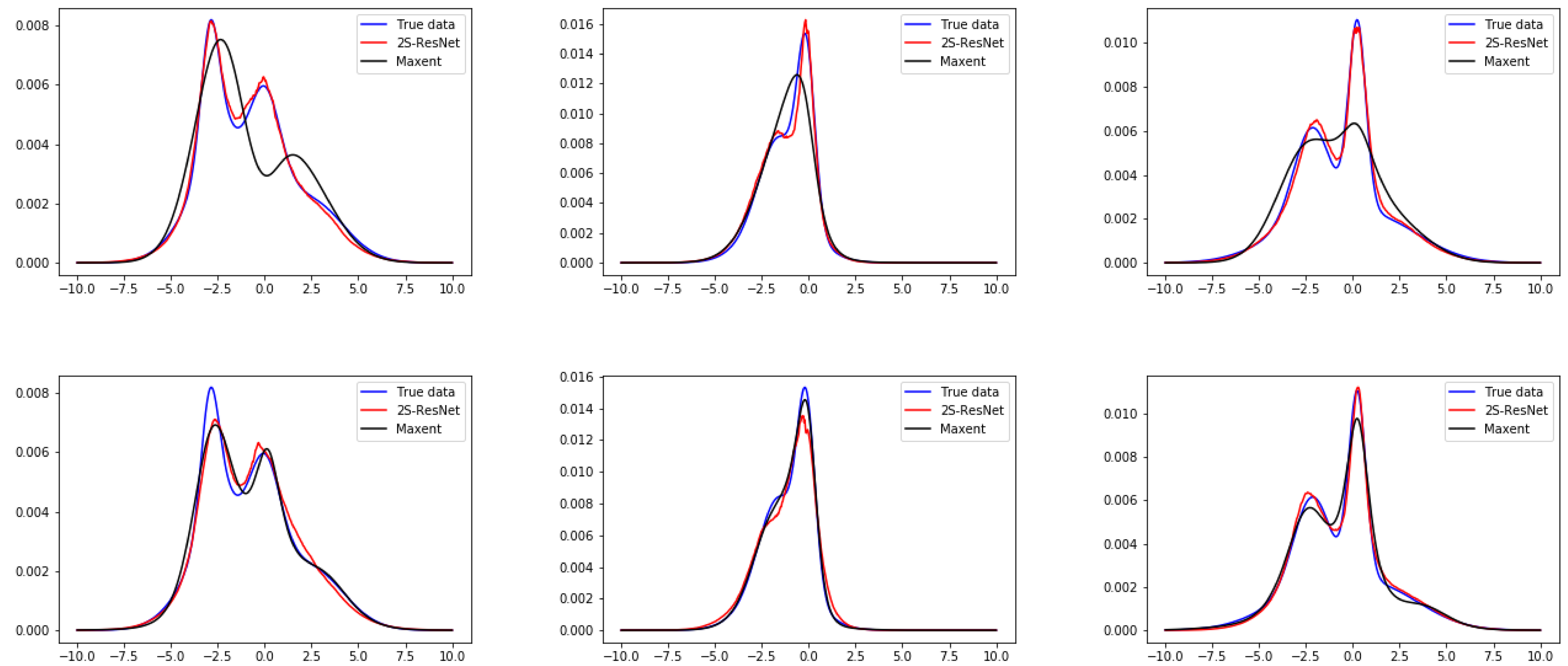
Dataset We generate the spectral densities $A(\omega)$ using a sum o f R uncorrelated Gaussian distributions:

$$A(\omega) = \frac{1}{R}\sum_{i=0}^{R} exp(-\frac{(\omega-\mu_i)^2}{2\sigma_i^2}) \tag{4}$$

Green's function can be computed via (1). 100k training dataset (A, G), 1000 samples for validation and test, respectively.

Numerical Experiment

Two step ResNet give better results than MaxEnt under high noise level.



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