Rational function regression method for numerical analytic continuation

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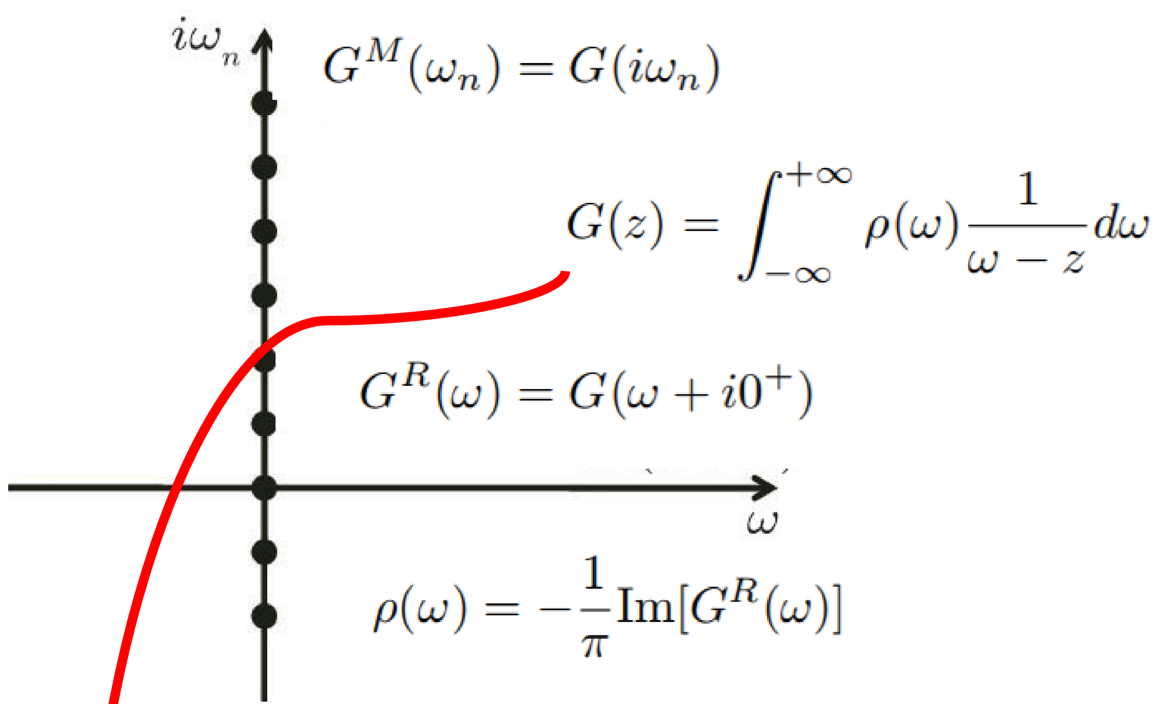
Background: Quantum Monte Carlo simulations



One of the bottlenecks of quantum Monte Carlo study is how to perform a reliable analytic continuation from imaginary time to real time. Two major families are the Padé method and the kernel based maximum entropy method. They both have their pros and cons. The Padé method needs very accurate imaginary time input data. The maximum entropy method requires a priori information.

The Method: Rational function and Linear Regression

$$G(z) = \frac{P_L(z)}{P_M(z)} = \frac{a_0 + a_1 z + \cdots + a_L z^L}{1 + b_1 z + \cdots + b_M z^M}$$

Polynomial Representation

There are N equations to be fit

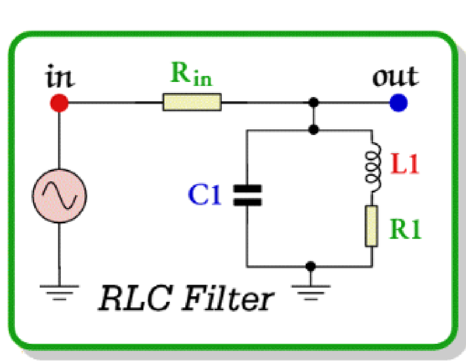
Zeros and poles $= a_0 \frac{(z - A_1)\cdots(z - A_L)}{(z - B_1)\cdots(z - B_M)}$

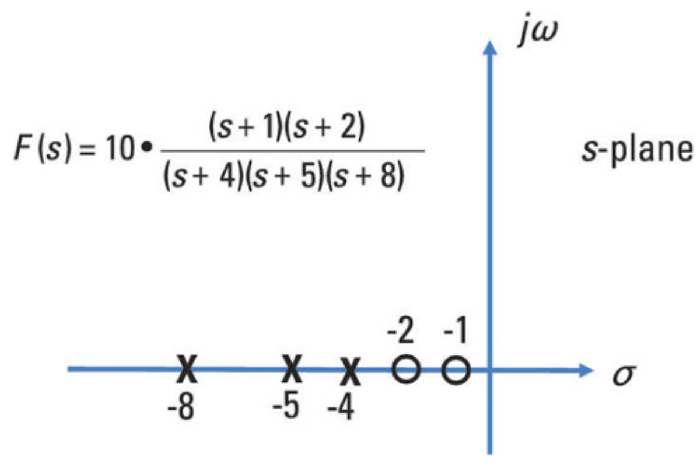
Residue number and poles $= \frac{R_1}{z - B_1} + \frac{R_2}{z - B_2} + \cdots + \frac{R_M}{z - B_M}$

$$\begin{pmatrix} -u_1 z_1^1 & -u_1 z_1^2 & \cdots & z_1^0 & z_1^1 & z_1^2 & \cdots \\ -u_2 z_2^1 & -u_2 z_2^2 & \cdots & z_2^0 & z_2^1 & z_2^2 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ -u_N z_N^1 & -u_N z_N^2 & \cdots & z_N^0 & z_N^1 & z_N^2 & \cdots \end{pmatrix} \begin{pmatrix} b_1 \\ b_2 \\ \vdots \\ a_0 \\ a_1 \\ a_2 \\ \vdots \end{pmatrix} = \begin{pmatrix} u_1 \\ u_2 \\ \vdots \\ u_{N-1} \\ u_N \end{pmatrix}$$

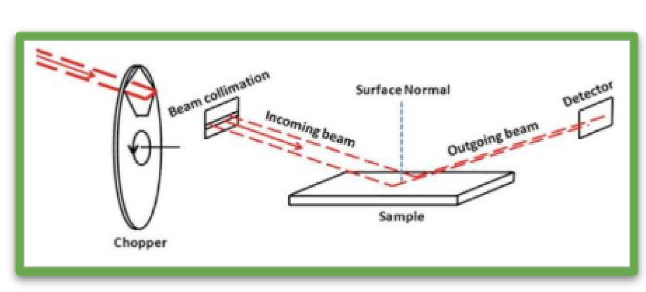
Rational function is the faithful representation of RCL circuit, therefore, we think it may be a good approximation for linear response system.

RLC circuits





Neutron scattering

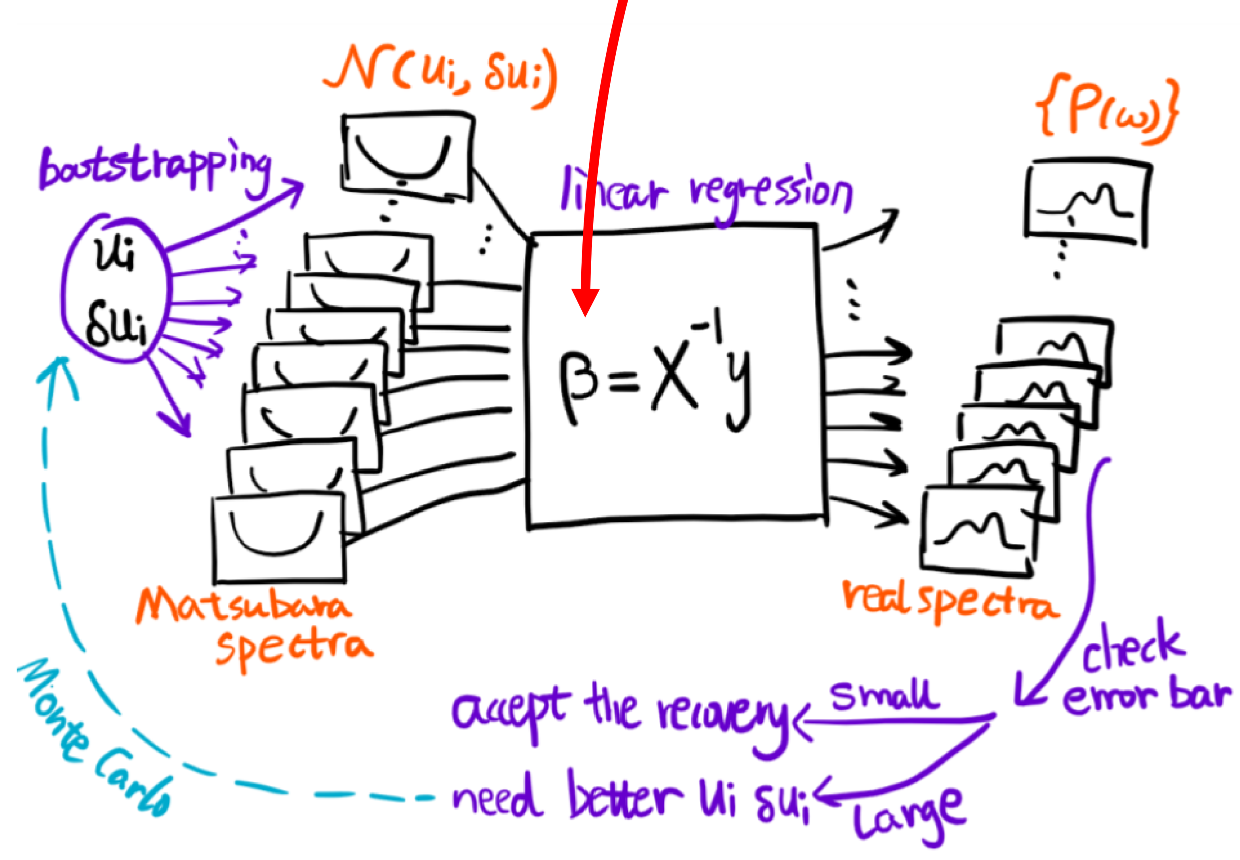


A linear regression problem

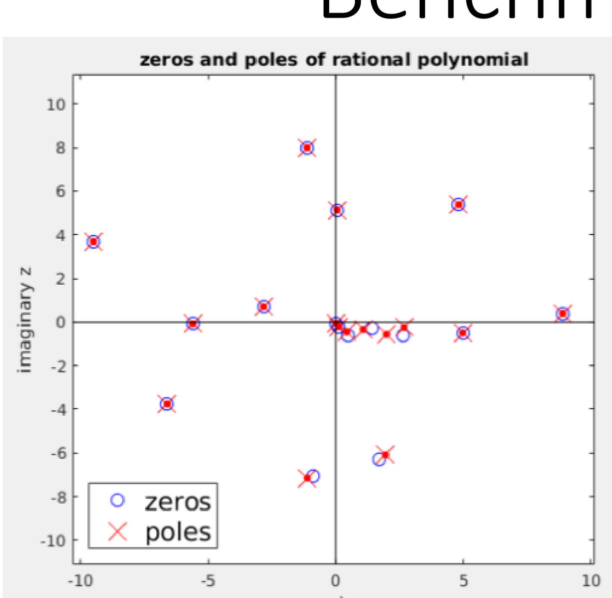
$$\mathbf{X}_{N\times(L+M+1)}\beta_{(L+M+1)} = \mathbf{y}_N$$

Find β that minimizes $||\mathbf{X}\beta - \mathbf{y}||^2$

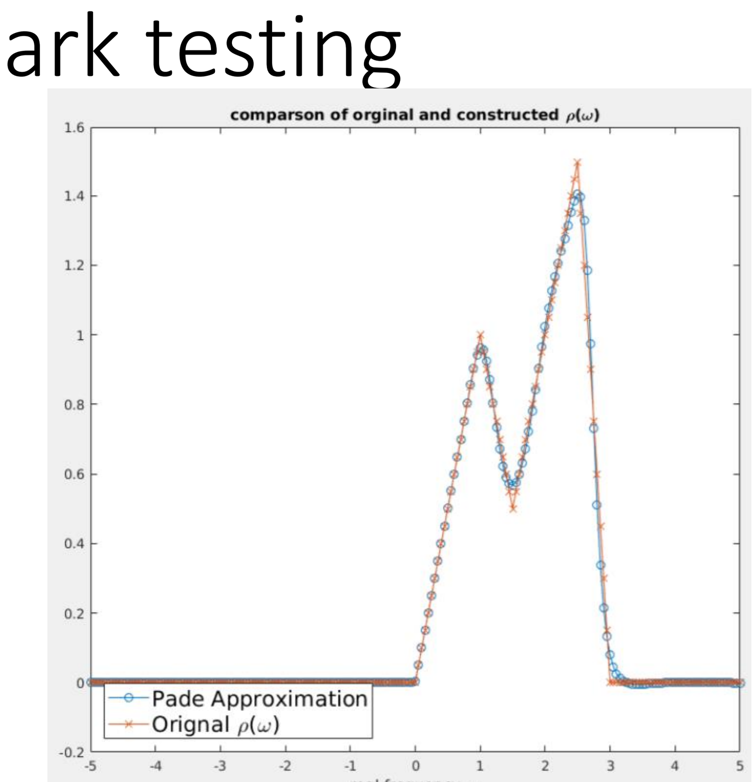
X and y comes from Monte Carlo simulation with error. We can use bootstrapping statistics to generate an ensemble of X and y, hence beta. So that we can estimate the error of beta.



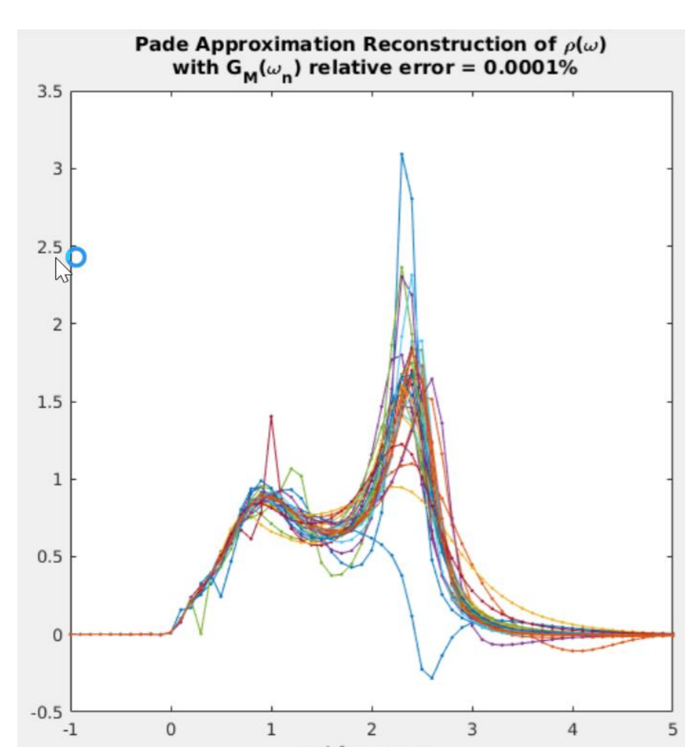
Benchmark testing



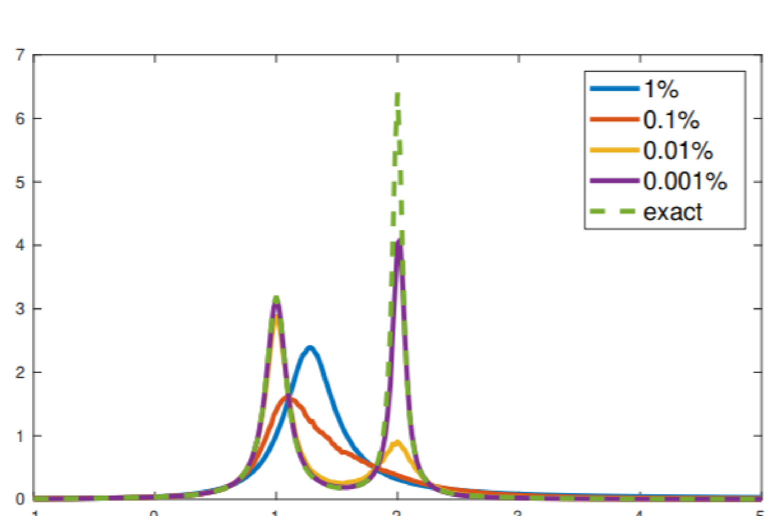
Zeros and poles



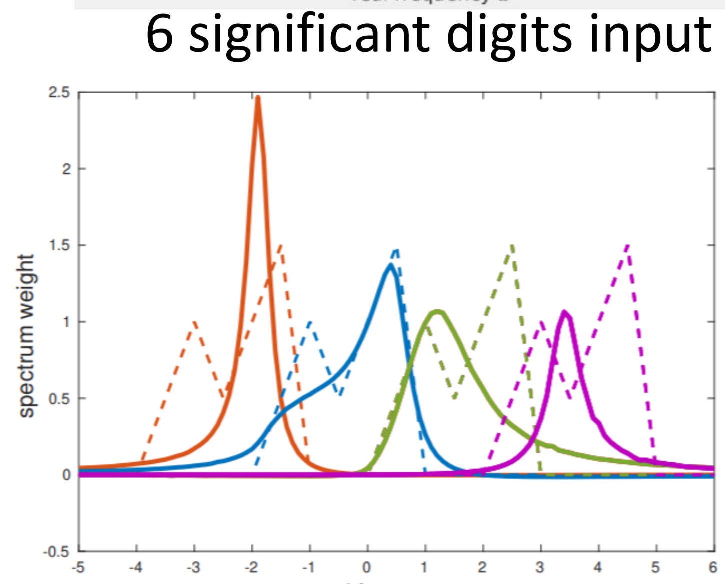
15 significant digits input



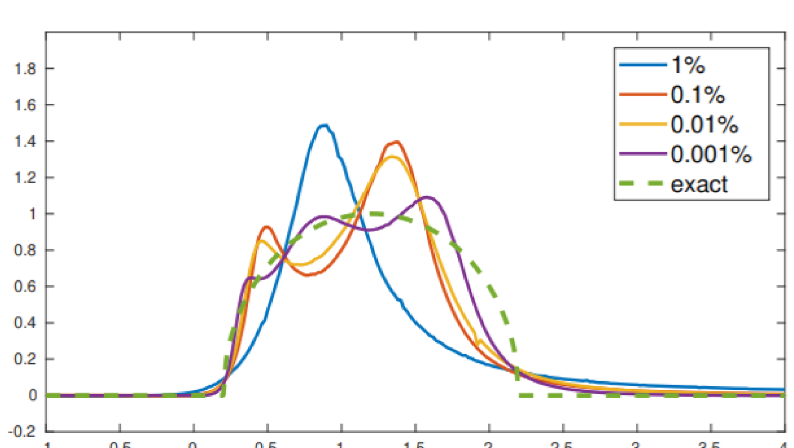
6 significant digits input



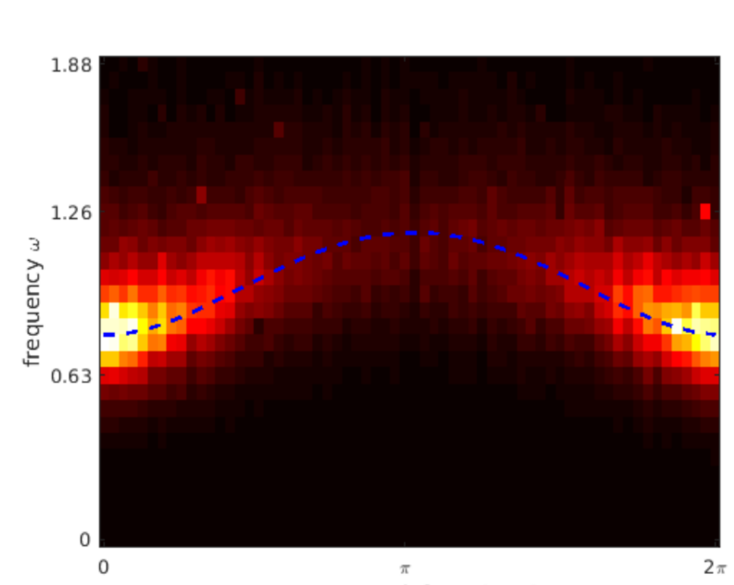
2,3,4,5 significant digits input.
Double Lorentz test function



2 significant digits input



2,3,4,5 significant digits input.
Semi-circle test function



Transverse field Ising model
Recovered from 4 significant digits Monte Carlo

Conclusion:

In this work we use rational function to represent the physical system. A matrix form is constructed, to convert it to a standard linear regression problem. Bootstrapping statistics is applied, to get best estimation and estimated errors. For high precision recovery, the error gives information about whether or not we need to increase the Monte Carlo data's accuracy. For low precision recovery, our method still gives correct position and amplitude of the spectrum even for 1% relative error input data. This regression form can be used for further study by utilizing the symmetry aspect of zeros and poles and the fully Bayesian choices of L and M