Note on power Lanczos method

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In this note, we show how to determine α in the power-Lanczos method. Within the finite-number sampling, it is important to use the decomposition that guarantees the positive definitive relation for variance. We also explain the sample perl scripts for calculating energy and variance after the single-step Lanczos method.

1. Determination of α

First, we briefly the sampling procedure of the variational Monte Carlo (VMC) method. Physical properties $\hat{A}$ are calculated as follows:

$$\langle\hat{A}\rangle = \frac{\langle\phi|\hat{A}|\phi\rangle}{\langle\phi|\phi\rangle} = \sum_x \rho(x)F(x,\hat{A}), \tag{1}$$

$$\rho(x) = \frac{|\langle\phi|x\rangle|^2}{\langle\phi|\phi\rangle} \qquad F(x,\hat{A}) = \frac{\langle x|\hat{A}|\phi\rangle}{\langle\phi|x\rangle}, \tag{2}$$

There is two ways to calculate the product of the operators $\hat{A}\hat{B}$.

$$\langle\hat{A}\hat{B}\rangle = \sum_x \rho(x)F(x,\hat{A}\hat{B}), \tag{3}$$

$$\langle\hat{A}\hat{B}\rangle = \sum_x \rho(x)F(\hat{A},x)F(x,\hat{B}). \tag{4}$$

As we explain later, in general, the latter way is numerical stable one. For example, we consider the expectation value of the variance, which is defined as $\sigma^2 = \langle(\hat{H} - \langle\hat{H}\rangle)^2\rangle$. There is two ways to calculate the variance.

$$\begin{aligned}\sigma^2 &= \frac{\sum_x\langle\phi|x\rangle\langle x|(\hat{H}-\langle\hat{H}\rangle)(\hat{H}-\langle\hat{H}\rangle)|\phi\rangle}{\langle\phi|\phi\rangle} \\ &= \sum_x \rho(x)F(x,\hat{H}^2) - \Big(\sum_x \rho(x)F(x,\hat{H})\Big)^2 \end{aligned} \tag{5}$$

$$\begin{aligned}\sigma^2 &= \frac{\sum_x\langle\phi|(\hat{H}-\langle\hat{H}\rangle)|x\rangle\langle x|(\hat{H}-\langle\hat{H}\rangle)|\phi\rangle}{\langle\phi|\phi\rangle} \\ &= \sum_x \rho(x)F(\hat{H},x)F(x,\hat{H}) - \Big(\sum_x \rho(x)F(x,\hat{H})\Big)^2. \end{aligned} \tag{6}$$

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From its definition, the latter way gives the positive definitive variance even for the finite sampling while the former way does not guarantee the positive definitiveness of the variance.

Here, we consider the expectation values of energy and variance for the (single-step) power Lanczos wave function $|\phi\rangle = (1+\alpha\hat{H})|\psi\rangle$. The energy is calculated as

$$\begin{aligned} E_{\mathrm{LS}}(\alpha) &= \frac{\sum_x \langle\psi|(1+\alpha\hat{H})|x\rangle\langle x|\hat{H}(1+\alpha\hat{H})|\psi\rangle}{\sum_x \langle\psi|(1+\alpha\hat{H})|x\rangle\langle x|(1+\alpha\hat{H})|\psi\rangle} \\ &= \frac{h_1 + \alpha(h_{2(20)} + h_{2(11)}) + \alpha^2 h_{3(12)}}{1 + 2\alpha h_1 + \alpha^2 h_{2(11)}}, \end{aligned} \tag{7}$$

where we define $h_{2(11)}$,$h_{2(20)}$, and $h_{3(12)}$ as

$$h_{2(11)} = \sum_x \rho(x) F(\hat{H}, x) F(x, \hat{H}), \tag{8}$$

$$h_{2(20)} = \sum_x \rho(x) F(\hat{H}^2, x), \tag{9}$$

$$h_{3(12)} = \sum_x \rho(x) F(\hat{H}, x) F(x, \hat{H}^2). \tag{10}$$

From the condition $\frac{\partial E_{\mathrm{LS}}(\alpha)}{\partial \alpha} = 0$, i.e., by solving the quadratic equations, we can determine the α (explicit form is given in the perl script). The variance is calculate in the similar way.

2. Perl scripts

By using Aft_SingleStepLanczos.pl, you can calculate the energy and variance of the power Lanczos method. Input files are ”zvo_aft_Lz_ls_00*.dat”. Outout files are ”Result_Lz.dat”, ”Lz_energy.dat”, and ”Lz_variance.dat”. In ”Result_Lz.dat”, the energy and variance are shown. In ”Lz_energy.dat” and ”Lz_variance.dat”, the α dependence of energy and variance are shown.