Extrapolation of diffusion Monte Carlo energies to zero time step

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Consider N DMC energies $\{e_1 \pm \sigma_{e_1}, \ldots, e_N \pm \sigma_{e_N}\}$ obtained at different time steps $\{\tau_1, \ldots, \tau_N\}$. Suppose the DMC energy as a function of time step can be written as

$$e(\tau) = \sum_{k=1}^{P} a_k \tau^{n_k}, \tag{1}$$

where the exponents $\{n_k\}$ are non-negative, but are not necessarily integers. One of the exponents must be zero: the coefficient of this term is the DMC energy at zero time step. The coefficients $\{a_k\}$ can be determined by minimizing the χ^2 function, where

$$\chi^2 = \sum_{i=1}^{N} \left(\frac{e_i - \sum_{k=1}^{P} a_k \tau_i^{n_k}}{\sigma_{e_i}} \right)^2. \tag{2}$$

By demanding that $\partial \chi^2 / \partial a_j = 0$, we find that

$$\sum_{k=1}^{P} \left(\sum_{i=1}^{N} \frac{\tau_i^{n_j+n_k}}{\sigma_{e_i}^2} \right) a_k = \sum_{i=1}^{N} \frac{e_i \tau_i^{n_j}}{\sigma_{e_i}^2}. \tag{3}$$

For $j, k \in \{1, \ldots, P\}$, let $M_{jk} \equiv \sum_{i=1}^{N} \tau_i^{n_j+n_k} / \sigma_{e_i}^2$ and $c_j \equiv \sum_{i=1}^{N} e_i \tau_i^{n_j} / \sigma_{e_i}^2$. Equation (3) can be written as $M\mathbf{a} = \mathbf{c}$ and hence we can find the vector of polynomial coefficients $\mathbf{a}$ by Gaussian elimination.

Note that the variance in a_j is approximately given by

$$\begin{aligned}
\sigma_{a_j}^2 &\approx \sum_{i=1}^{N} \sigma_{e_i}^2 \left(\frac{\partial a_j}{\partial e_i} \right)^2 \\
&= \sum_{i=1}^{N} \sigma_{e_i}^2 \left(\sum_{k=1}^{P} M_{jk}^{-1} \frac{\tau_i^{n_k}}{\sigma_{e_i}^2} \right)^2 \\
&= \sum_{k=1}^{P} \sum_{l=1}^{P} M_{jk}^{-1} M_{jl}^{-1} \sum_i \frac{\tau_i^{n_k+n_l}}{\sigma_{e_i}^2} = \sum_{k=1}^{P} \sum_{l=1}^{P} M_{jk}^{-1} M_{jl}^{-1} M_{kl} = M_{jj}^{-1}.
\end{aligned} \tag{4}$$

This gives an estimate of the standard errors in the fitted polynomial coefficients.

The utility EXTRAPOLATE_TAU carries out these calculations numerically. To use this utility, first prepare a text file with three columns of data: the time steps, the DMC energies and the standard errors in the DMC energies, respectively. Then type *extrapolate_tau* and follow the instructions.