Quasi-sparse eigenvector diagonalization and stochastic error correction

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Abstract

We briefly review the diagonalization of quantum Hamiltonians using the quasi-sparse eigenvector (QSE) method. We also introduce the technique of stochastic error correction, which systematically removes the truncation error of the QSE result by stochastically sampling the contribution of the remaining basis states.

1 Quasi-sparse eigenvector method

Quasi-sparse eigenvector (QSE) diagonalization is a new computational method which finds approximate low-lying eigenvalues and eigenvectors for a general quantum field Hamiltonian $H$ [1]. It handles the exponential increase in the dimension of Fock space by exploiting the sparsity of the Hamiltonian. The method is most effective when the splitting between low-lying eigenvalues is not too small compared to the size of the Hamiltonian off-diagonal entries. In such cases the low-lying eigenvectors are quasi-sparse, meaning that the vector is dominated by a small fraction of its largest components. The QSE algorithm is applied using the following steps:

1. Select a subset of orthonormal basis vectors $\{e_{i_1}, \ldots, e_{i_n}\}$ and call the corresponding subspace $S$.
2. Diagonalize $H$ restricted to $S$ and find one eigenvector $v$.
3. Sort the basis components $\langle e_{i_j} | v \rangle$ according to their magnitude and remove the least important basis vectors.
4. Replace the discarded basis vectors by new basis vectors. These are selected at random from a pool of candidate basis vectors which are connected to the old basis vectors through non-vanishing matrix elements of $H$.
5. Redefine $S$ as the subspace spanned by the updated set of basis vectors and repeat steps 2 through 5.
If the subset of basis vectors is sufficiently large, the exact low energy eigen-

vectors will be stable fixed points of the QSE update process. We can show

t this as follows. Let $|i\rangle$ be the eigenvectors of the submatrix of $H$ restricted to

the subspace $S$, where $S$ is the span of the subset of basis vectors after step 3

of the QSE algorithm. Let $|A_j\rangle$ be the remaining orthonormal basis vectors

in the full space not contained in $S$. We can represent $H$ as

$$
\begin{bmatrix}
\lambda_1 & 0 & \cdots & \langle 1 | H | A_1 \rangle & \langle 1 | H | A_2 \rangle & \cdots \\
0 & \lambda_2 & \cdots & \langle 2 | H | A_1 \rangle & \langle 2 | H | A_2 \rangle & \cdots \\
\vdots & \vdots & \ddots & \vdots & \vdots & \cdots \\
\langle A_1 | H | 1 \rangle & \langle A_1 | H | 2 \rangle & \cdots & E \cdot \lambda_{A_1} & \langle A_1 | H | A_2 \rangle & \cdots \\
\langle A_2 | H | 1 \rangle & \langle A_2 | H | 2 \rangle & \cdots & \langle A_2 | H | A_1 \rangle & E \cdot \lambda_{A_2} & \cdots \\
\vdots & \vdots & \vdots & \vdots & \vdots & \ddots
\end{bmatrix}.
$$

(1)

We have written the diagonal terms for the basis vectors $|A_j\rangle$ with an explicit

factor $E$ for reasons to be explained shortly. We let $|1\rangle$ be the approximate
eigenvector of interest and shift the diagonal entries so that $\lambda_1 = 0$. Our

starting hypothesis is that $|1\rangle$ is close to some exact eigenvector of $H$ which

we denote as $|1_{\text{full}}\rangle$. More precisely we assume that the components of $|1_{\text{full}}\rangle$

outside $S$ are small enough so that we can expand in inverse powers of the

introduced parameter $E$.

We now expand the eigenvector as

$$
|1_{\text{full}}\rangle = \begin{bmatrix}
1 + \cdots \\
c'_2 E^{-1} + \cdots \\
\vdots \\
c'_{A_1} E^{-1} + \cdots \\
c'_{A_2} E^{-1} + \cdots \\
\vdots
\end{bmatrix}
$$

(2)

and the corresponding eigenvalue as

$$
\lambda_{\text{full}} = \lambda'_1 E^{-1} + \cdots.
$$

(3)

In (2) we have constrained $|1_{\text{full}}\rangle$ to have unit norm. From the eigenvalue

equation $H |1_{\text{full}}\rangle = \lambda_{\text{full}} |1_{\text{full}}\rangle$ we find at lowest order

$$
c'_{A_j} = -\frac{\langle A_j | H | 1 \rangle}{\lambda'_{A_j}}.
$$

(4)
We see that at lowest order the component of $|1\text{full}\rangle$ in the $|A_j\rangle$ direction is independent of the other vectors $|A_{j'}\rangle$. If $|1\rangle$ is sufficiently close to $|1\text{full}\rangle$ then the limitation that only a fixed number of new basis vectors is added in step 4 of the QSE algorithm is not important. At lowest order in $E^{-1}$ the comparison of basis components in step 3 (in the next iteration) is the same as if we had included all remaining vectors $|A_j\rangle$ at once. Therefore at each update only the truly largest components are kept and the algorithm will converge to some optimal approximation of $|1\text{full}\rangle$. This is consistent with the actual performance of the algorithm for a wide range of examples.

2 Stochastic error correction

The quasi-sparse eigenvector method approximates the low energy eigenvalues and eigenvectors of a Hamiltonian $H$ by finding and diagonalizing optimized subspaces $S$. This procedure however has an intrinsic error due to the omission of basis states not in $S$. The goal of stochastic error correction is to sample the contribution of these remaining basis vectors in a systematic fashion. Due to space limitations we consider here only the series expansion method. Several other techniques are discussed in a forthcoming paper [2].

The series method for stochastic error correction is based on the $E^{-1}$ expansion introduced in the previous section,}

$$|1\text{full}\rangle \propto \begin{bmatrix} 1 \\ c_2E^{-1} + c_2' E^{-2} + \cdots \\ \vdots \\ c_{A_1}E^{-1} + c_{A_1}' E^{-2} + \cdots \\ c_{A_2}E^{-1} + c_{A_2}' E^{-2} + \cdots \\ \vdots \end{bmatrix},$$

(5)

$$\lambda_{\text{full}} = \lambda_1' E^{-1} + \lambda_1'' E^{-2} \cdots.$$  

(6)

This time it is more convenient to choose the normalization of the eigenvector such that the $|1\rangle$ component remains 1. The convergence of the expansion is controlled by the proximity of $|1\rangle$ to $|1\text{full}\rangle$. If $|1\rangle$ is not at all close $|1\text{full}\rangle$ then it will be necessary to use a more robust method, and such methods are discussed in [2].
At first order in $E^{-1}$ we find

\[ c'_{A_j} = -\frac{\langle A_j | H | 1 \rangle}{\lambda_{A_j}} \] (7)

\[ \lambda'_1 = -\sum_j \frac{\langle 1 | H | A_j \rangle \langle A_j | H | 1 \rangle}{\lambda_{A_j}} \] (8)

\[ c'_j = \frac{1}{\lambda_j} \sum_k \frac{\langle j | H | A_k \rangle \langle A_k | H | 1 \rangle}{\lambda_{A_k}}. \] (9)

The second order contributions are

\[ c''_{A_j} = \sum_{k \neq j} \frac{\langle A_j | H | A_k \rangle \langle A_k | H | 1 \rangle}{\lambda_{A_j} \lambda_{A_k}} - \sum_{l \neq 1} \sum_k \frac{\langle A_j | H | l \rangle \langle l | H | A_k \rangle \langle A_k | H | 1 \rangle}{\lambda_{A_j} \lambda_l \lambda_{A_k}} \] (10)

\[ \lambda''_1 = \sum_j \sum_{k \neq j} \frac{\langle 1 | H | A_j \rangle \langle A_j | H | A_k \rangle \langle A_k | H | 1 \rangle}{\lambda_{A_j} \lambda_{A_k}} - \sum_j \sum_{l \neq 1} \sum_k \frac{\langle 1 | H | A_j \rangle \langle A_j | H | l \rangle \langle l | H | A_k \rangle \langle A_k | H | 1 \rangle}{\lambda_{A_j} \lambda_l \lambda_{A_k}} \] (11)

\[ c''_m = -\sum_j \sum_{k \neq j} \frac{\langle m | H | A_j \rangle \langle A_j | H | A_k \rangle \langle A_k | H | 1 \rangle}{\lambda_m \lambda_{A_j} \lambda_{A_k}} \] (12)

\[ + \sum_j \sum_{l \neq 1} \sum_k \frac{\langle m | H | A_j \rangle \langle A_j | H | l \rangle \langle l | H | A_k \rangle \langle A_k | H | 1 \rangle}{\lambda_m \lambda_{A_j} \lambda_l \lambda_{A_k}} \]

\[ - \frac{1}{\lambda_m} \left[ \sum_j \frac{\langle 1 | H | A_j \rangle \langle A_j | H | 1 \rangle}{\lambda_{A_j}} \right] \frac{1}{\lambda_m} \left[ \sum_k \frac{\langle m | H | A_k \rangle \langle A_k | H | 1 \rangle}{\lambda_{A_k}} \right]. \]

These contributions are calculated by a Monte Carlo sampling process. Let $P(A_{\text{trial}(i)})$ denote the probability of selecting $A_{\text{trial}(i)}$ on the $i$th trial. For example the first order correction to the eigenvalue can be calculated using

\[ \lambda'_1 = -\sum_j \frac{\langle 1 | H | A_j \rangle \langle A_j | H | 1 \rangle}{\lambda_{A_j}} \] (13)

\[ = -\lim_{N \to \infty} \frac{1}{N} \sum_{i=1, \ldots, N} \frac{\langle 1 | H | A_{\text{trial}(i)} \rangle \langle A_{\text{trial}(i)} | H | 1 \rangle}{\lambda_{A_{\text{trial}(i)}} P(A_{\text{trial}(i)})}. \] (14)

Application of the series method for stochastic error correction to the Hubbard model was discussed by Nathan Salwen at the Heidelberg meeting and is presented in another article in these proceedings.
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References

[1] D. J. Lee, N. Salwen, D. D. Lee, hep-th/0002251.

[2] D. Lee, N. Salwen, M. Windoloski, work in progress.