Daigonalization of large matrices Davidson procedure Metod to obtain a few eigenvalues and corresponding eigenvectors

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Diagonalization - Davidson procedure

To avoid confusion I assume the following convention:

- **Square matrices** are denoted with **red color**, e.g. $\mathbf{A}$, $\tilde{\mathbf{A}}$
- **Vectors** (i.e., one-column matrices) are indicated with **blue color**, e.g. $\mathbf{b_i}$, $\mathbf{c_i}$, $\mathbf{d_i}$, $\mathbf{e_i}$, $\mathbf{x_i}$, $\mathbf{y_i}$
- **Numbers** (i.e., elements of matrices) are denoted with **black ink**, e.g. $\mathbf{A_{ri}}$, $\mathbf{b_{ri}}$, $\alpha_{\mathbf{ri}}$

Diagonalization - Davidson procedure

A - matrix to be diagonalized

We need a starting vector: $\mathbf{b}(\text{begin})=\mathbf{b_o}$

Then:

in each iteration we construct (according to **Davidson presciption**) a new vector $\mathbf{b_i}$ and

Diagonalization - Davidson procedure

in each iteration we construct the vector **c** which is an approximation to the true eigenvector of the **matrix A** as
a linear combination of all — so far constructed — vectors **b**:

$$\mathbf{c} = \sum_{\mathbf{r}} \alpha_{\mathbf{r}} \mathbf{b}_{\mathbf{r}}$$

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The main idea in the Davidson approach is a construction of the small matrix $\tilde{\mathbf{A}}$ the elements of which are given with the formula

$$\tilde{a}_{ij} = \langle b_i | x_i \rangle$$

where

$$x_i = A b_i$$

Diagonalization - Davidson procedure

Thus the general scheme of finding the approximate eigenvalues and eigenvectors of the **A matrix** is following:

- having **n** vectors $\{\mathbf{b_1}, \mathbf{b_2} \cdots \mathbf{b_n}\}$
- we construct the **n** vectors $\{\mathbf{x_1}, \mathbf{x_2} \cdots \mathbf{x_n}\}$
- then we build the **matrix** $\tilde{\mathbf{A}}$ with the prescription:

$$\tilde{\mathbf{a}}_{\mathbf{ij}} = \langle \mathbf{b_i} | \mathbf{x_i} \rangle$$

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Construction of the Davidson vector:

if the vector $\mathbf{c_i}$ is an eigenvector of matrix A then it should fullfil the eigenvalue equation:

$$\mathbf{A c_i} = \lambda_\mathbf{i} \mathbf{c_i}$$

or

$$\mathbf{A c_i} - \lambda_\mathbf{i} \mathbf{c_i} = \mathbf{0}$$

If $\lambda_\mathbf{i}$ and $\mathbf{c_i}$ are approximate solution of the eigenvalue equation then we may define the error vector $\mathbf{e_i}$ as

$$\mathbf{e_{ri}} = \mathbf{y_{ri}} - \lambda_\mathbf{i} \mathbf{c_{ri}} = \mathbf{0}$$

where

$$\mathbf{y_i} = \mathbf{A c_i}$$

Diagonalization - Davidson procedure

If the error vector is equal zero or its norm is below some treshold we may consider the eigenvalue equation fullfilled and the eigenvalue problem solved. If not then construct the Davidson vector $\mathbf{d_i}$

$$\mathbf{d_{ri}} = \mathbf{e_{ri}}/(\lambda_\mathbf{i} - \mathbf{A_{rr}})$$

The $\mathbf{d_i}$ vector after being orthogonalized to the existing n vectors $\{\mathbf{b_i}\}$ is used to increase by one the size of the subspace spanned by the vectors $\{\mathbf{b_i}\}$, i.e. it becomes a vector $\mathbf{b_{n+1}}$.

Diagonalization - Davidson procedure

A crucial step in the EOM-CC calculations

$$\mathbf{x}_k = \mathbf{A}\mathbf{b}_k$$

Why?

Because the **A matrix** is not known!

Rank of **A** goes into milions.

E.g., for N_2 with **aug-cc-pVQZ** basis set at the **EOM-CCSDT** level is equal to:

107 799 210