Preface

Computational methods in quantum chemistry often require an extensive handling of large matrices. As such, fundamental linear algebra techniques are necessary for solving eigenvalue problems like the Schrödinger equation.

$$\hat{H}\Psi = E\Psi \tag{1}$$

Diagonalization

Diagonalization involves converting a square matrix into a diagonal matrix constructed from its eigenvalues and finding the eigenvectors that correspond to those eigenvalues. A matrix is considered diagonalizable if the following expression holds:

$$A = V\Lambda V^{-1} \tag{2}$$

Where V is the eigenvector matrix of A and V^{-1} is its inverse. Λ is a diagonal matrix with diagonal elements corresponding to the eigenvalues of A.

You can compute the inverse of V using the following:

$$V^{-1} = \frac{1}{|V|} adj(V) \tag{3}$$

$|V|$ is the determinant of V and $adj(V)$ is the adjugate of V or the transpose of the cofactor matrix of V.

A general eigensystem $A\nu = \lambda\nu$ may be solved if $(A - \lambda I)$ is invertible. λ represents the eigenvalues, ν is the set of eigenvectors, and I is the identity matrix. The eigenvalues may be obtained by taking the determinant of $(A-\lambda I)$ and solving the characteristic polynomial of A (i.e. finding the roots). The corresponding eigenvectors may be obtained by matching the column-wise elements of ν with the row-wise elements of $(A - \lambda I)$.

$$(A - \lambda I)\nu = 0 \tag{4}$$

Singular Value Decomposition (SVD)

Singular Value Decomposition (SVD) *decomposes A, an $(m \times n)$ matrix, into three factors: U, Σ, and V^T.*

$$A = U\Sigma V^T \tag{5}$$

- U is an orthogonal matrix of size $(m \times m)$.
- Σ is a diagonal matrix composed of the singular values with a dimensionality of $(m \times n)$. The singular values are the square roots of non-negative eigenvalues of the self-adjoint operator $A^\dagger A$ or $A^T A$ for reals. $A^T A$ is a Hermitian matrix with linearly independent eigenvectors and real eigenvalues. The eigenvalues of a linear Hermitian operator can describe quantum observables.
- V^T is an orthogonal matrix of size $(n \times n)$ that is constructed from the normalized eigenvectors of A. For normalization, each scalar component is divided by the norm of the vector.
- Orthogonal matrices are necessarily invertible and unitary (i.e. $U^T U = UU^T = I$ and $V^T V = VV^T = I$).

Suzuki-Trotter Approximation

Trotterization *involves the decomposition of Hamiltonian operators for n-qubits or quantum subsystems. This method makes quantum simulations for approximating the full time-evolution Hamiltonian more tractable. This is a very basic description of the Trotter method and its application within quantum computing for quantum chemistry. Simply put, the Suzuki-Trotter approximation is based on the Lie product formula for an exponential ansatz (e.g. Unitary Coupled Cluster). If operators $\hat{A}$ and $\hat{B}$ do not commute, the following can be approximated:*

$$e^{\hat{A}+\hat{B}} \approx e^{\hat{A}} e^{\hat{B}} \tag{6}$$

Which becomes exact at infinite order:

$$e^{\hat{A}+\hat{B}} = \lim_{n\to\infty} \left(e^{\frac{\hat{A}}{n}} e^{\frac{\hat{B}}{n}} \right)^n \tag{7}$$

Thus, the computational cost for diagonalizing a factorized system of matrices may be reduced. Variational quantum eigensolvers (VQEs) are currently being developed to find variational solutions to eigenvalue and optimization problems that cannot be efficiently obtained using classical computers.

Selected Exercises

1. Diagonalize matrix A and show that $A = V\Lambda V^{-1}$ holds.

$$A = \begin{bmatrix} 6 & 3 \\ -4 & -1 \end{bmatrix}$$

2. Using SVD, decompose matrix Z into U, Σ, and V^T and show that $Z = U\Sigma V^T$ holds.

$$Z = \begin{bmatrix} 2 & 0 \\ 1 & 3 \end{bmatrix}$$