# Alternating algorithm for the nonsymmetric eigenvalue problems with tensor trains: application to quantum chemistry

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**Duration** : 6 months (between February and September 2026) with a possible continuation into a PhD.

**Keywords** : tensor trains, nonsymmetric eigenvalue problems, numerical linear algebra.

## 1 Motivation

In high-dimensional problems, tensor decompositions provide an efficient means to reduce the complexity of the objects being handled. In physics and chemistry, tensors naturally arise from many-body problems, whose solution give crucial information on the properties of the system.

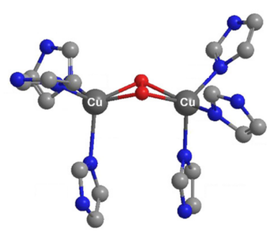

Figure 1: Oxytyrosinase

For an $N$-electron state, the electronic wave function $u : \mathbb{R}^{3N} \to \mathbb{R}$ solves the *so-called* Schrödinger equation, which is the linear eigenvalue problem

$$Hu = Eu, \tag{1}$$

where $E$ is the lowest eigenvalue of $H$, called the *electronic Hamiltonian*, defined by

$$H = \sum_{i=1}^{N} -\frac{1}{2}\Delta_{r_i} + v(r_i) + \sum_{i \neq j} \frac{1}{|r_i - r_j|}, \quad \text{and } v(r) = \sum_{k=1}^{N_{\text{nuc}}} -\frac{Z_k}{|r - R_k|}.$$

The Galerkin discretisation of the continuous eigenvalue problem involves a tensorised basis which gives a poor description of the electron-electron interaction. Because of the Coulomb interaction, the electronic wave function behaves like $u(r_1, r_2, \cdot) \sim |r_1 - r_2|(\frac{1}{2} + o(1))$ for $r_1$ close to $r_2$. This behaviour is universal and has been rigorously established for electronic Hamiltonians (Fournais et al. 2005). Tensorised basis of the form $(\phi_i(r_1)\phi_j(r_2))_{ij}$ shows a slow convergence to $|r_1 - r_2|$, especially close to the derivative singularity at $r_1 = r_2$ (Friesecke 2003).

Transcorrelation (TC) is a method designed to tackle this difficulty. TC methods incorporate this universal behaviour by factorising the wave function with a scalar function of the form $e^T$. It is not advisable to work in the Galerkin approximation of the form $(e^T \Phi_k)$, where $(\Phi_k)$ are tensorised, as the overlap matrix $e^{2T}$ is extremely expensive to compute. Instead, in TC an equivalent eigenvalue problem to (Equation 1) is solved which is

$$e^{-T} H e^T v = Ev,$$

{eq-TC_eigval_pb} where the original wave function can be retrieved by $u = e^T v$. The main drawback in TC is that the matrix $e^{-T} H e^T$ is not anymore Hermitian.

## 2 Non-symmetric alternating linear scheme

In the past decades, a new method has emerged, called *density-matrix renormalisation group* (DMRG) (White 1992) in physics, relying on a specific tensor format known as *tensor trains* (TT) (Oseledets 2011). In the mathematics community, the DMRG procedure is better known as *alternating linear scheme* (ALS).

The starting point of the ALS procedure is to write the eigenvector $u \in \mathbb{R}^{n_1 \times \dots \times n_d}$ as a TT $(A_k)_{1 \leq k \leq d}$, where for each $1 \leq i_k \leq n_k$, $A_k[i_k] \in \mathbb{R}^{r_{k-1} \times r_k}$ and for all $i_1, \dots, i_d$

$$u_{i_1 \dots i_d} = A_1[i_1] \cdots A_d[i_d].$$

Using a TT parametrisation $(A_1, \dots, A_d)$ for $u$ and the Rayleigh-Ritz characterisation of the lowest eigenvalue problem, the symmetric eigenvalue problem can be solved by an alternating optimisation over each TT core $A_k$. This optimisation problem for each TT core has a low cost, as the dimension of the TT core is much smaller than in the original problem. Moreover it is again quadratic, thus one can exploit standard numerical linear algebra tools to solve it.

The extension of the ALS to nonsymmetric eigenvalue problems requires to understand how to handle low-rank approximations of left and right eigenvectors. Extending the ALS to nonsymmetric eigenvalue problems necessitates addressing the low-rank approximation of both left and right eigenvectors. The two primary challenges involve assessing the accuracy of the eigenvalue and right eigenvector in relation to rank truncation, and ensuring the stability of the biorthogonalisation process between left and right eigenvectors.

## 3 Scientific program

1. Develop a stable nonsymmetric ALS in a two-dimensional case.
2. Analyse the convergence of the nonsymmetric ALS in the 2D setting.
3. Extension of the algorithm and the analysis to the tensor train case.

## References


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