Journal of Computational Physics 302 (2015) 329–335

Contents lists available at ScienceDirect

Journal of Computational Physics

www.elsevier.com/locate/jcp

Short note

# Compression of the electron repulsion integral tensor in tensor hypercontraction format with cubic scaling cost

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ARTICLE INFO

*Article history:*
Received 15 December 2014
Received in revised form 17 June 2015
Accepted 11 September 2015
Available online 15 September 2015

*Keywords:*
Electronic structure
Tensor compression
Column selection
Coulomb repulsion integral

ABSTRACT

Electron repulsion integral tensor has ubiquitous applications in electronic structure computations. In this work, we propose an algorithm which compresses the electron repulsion tensor into the tensor hypercontraction format with $\mathcal{O}(nN^2 \log N)$ computational cost, where $N$ is the number of orbital functions and $n$ is the number of spatial grid points that the discretization of each orbital function has. The algorithm is based on a novel strategy of density fitting using a selection of a subset of spatial grid points to approximate the pair products of orbital functions on the whole domain.



## 1. Introduction

Given a set of orbital functions $\{\psi_i\} \subset L^2(\mathbb{R}^3)$, the four-center two-electron repulsion integrals

$$(ij|kl) = \iint_{\mathbb{R}^3 \times \mathbb{R}^3} \frac{\psi_i(x)\psi_j(x)\psi_k(y)\psi_l(y)}{|x-y|}\,\mathrm{d}x\,\mathrm{d}y \tag{1}$$

are universally used in many electronic structure theories, such as Hartree–Fock, density functional theory (DFT), RPA, MP2, CCSD, and GW. As a result, a key step to accelerate ab initio computations in quantum chemistry and materials science is to get an efficient representation of the electron repulsion integral tensor.

One of the most popular methods for compressing the electron repulsion integral is the density fitting approximation. This method, also known as resolution of identity approach [3,18,19,22,24,25], amounts to representing pair products of orbital functions $\psi_i(x)\psi_j(x)$ in terms of a set of auxiliary basis functions

$$\rho_{ij}(x) := \psi_i(x)\psi_j(x) \approx \widetilde{\rho}_{ij}(x) = \sum_{\mu} C_{ij}^{\mu} P_{\mu}(x), \tag{2}$$

where $\mu = 1, 2, \ldots, N_{\mathrm{aux}}$ labels the auxiliary basis functions. The auxiliary basis functions are constructed either explicitly (e.g., a set of Gaussian-type atom-centered basis functions) or implicitly by using singular value decomposition on the overlap matrix of the set of $N^2$ functions $\rho_{ij}(x)$ [4,5].

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http://dx.doi.org/10.1016/j.jcp.2015.09.014
0021-9991/

After the auxiliary basis functions are determined, a least square fitting is used to determine the coefficient $C_{ij}^{\mu}$. When the standard $L^2$ metric is used in the least square fitting, one obtains

$$C_{ij}^{\mu} = \sum_{\nu} \langle ij|\nu\rangle S_{\nu\mu}^{-1}, \tag{3}$$

$$(ij|kl) \approx \sum_{\mu\mu'\nu\nu'} \langle ij|\nu\rangle S_{\nu\mu}^{-1} V_{\mu\mu'} S_{\mu'\nu'}^{-1} \langle \nu'|kl\rangle \tag{4}$$

with the shorthand notations

$$\langle ij|\nu\rangle = \int \psi_i(x)\psi_j(x)P_\nu(x)\,\mathrm{d}x, \tag{5}$$

$$S_{\mu\nu} = \int P_\mu(x)P_\nu(x)\,\mathrm{d}x, \qquad \text{and} \tag{6}$$

$$V_{\mu\nu} = \iint \frac{P_\mu(x)P_\nu(y)}{|x-y|}\,\mathrm{d}x\,\mathrm{d}y. \tag{7}$$

It is also possible to use the Coulomb weight in the least square fitting, which leads to

$$C_{ij}^{\mu} = \sum_{\nu} (ij|\nu) V_{\nu\mu}^{-1}, \tag{8}$$

$$(ij|kl) \approx \sum_{\mu\nu} (ij|\mu) V_{\mu\nu}^{-1} (\nu|kl) \tag{9}$$

with the shorthand notation

$$(ij|\nu) = \iint \frac{\psi_i(x)\psi_j(x)P_\nu(y)}{|x-y|}\,\mathrm{d}x\,\mathrm{d}y. \tag{10}$$

A closely related idea to density fitting is the incomplete Cholesky decomposition of the electron repulsion integrals [1,11]:

$$(ij|kl) \approx \sum_{\mu=1}^{M} L_{ij}^{\mu} L_{kl}^{\mu}, \tag{11}$$

where $L_{ij}^{\mu}$ are numerically obtained Cholesky vectors. The cost of getting the resolution of identity approximation, assuming $\mathcal{O}(N)$ auxiliary basis functions, is $\mathcal{O}(N^4)$, where $N$ is the number of orbital functions. Other methods for the electron repulsion integral tensor include multipole moment approaches [8,23,26,27] and pseudospectral representation [6,13,14].

More recently, the tensor hypercontraction of the electron repulsion integral have been proposed in [10,15,17], which aims at an approximation of the electron repulsion integral tensor as

$$(ij|kl) \approx \sum_{\mu\nu} X_i^{\mu} X_j^{\mu} Z^{\mu\nu} X_k^{\nu} X_l^{\nu}, \tag{12}$$

where $\mu, \nu$ are the indices for the decomposition. The factor $X$ is taken to be the weighted collocation matrix arises from numerical quadrature of the electron repulsion integral and $Z$ is determined by a least square procedure. The computational cost of obtaining the approximation is either $\mathcal{O}(N^5)$ when direct quadrature of electron repulsion integral is used or $\mathcal{O}(N^4)$ with the help of density fitting procedure. The tensor hypercontraction opens doors to efficient algorithms for several electronic structure theories, see e.g., [9,10,16,17,20,21].

In this work, we propose an $\mathcal{O}(nN^2 \log N)$ algorithm to get the tensor hypercontraction of the electron repulsion integral. It is based on an approximation of $\rho_{ij}(x)$ similar to (2), but with the key advantage that the coefficient $C_{ij}^{\mu}$ has separate dependence on the indices $i$ and $j$. Such an approximation is achieved by an interpolative decomposition which chooses selected grid points $x_\mu$ to interpolate the pair product density $\rho_{ij}$. This is different from the usual density fitting strategy with a predetermined set of auxiliary basis functions. In this sense, our algorithm tries to find an optimal set of the auxiliary basis functions, such that the tensor hypercontraction format can be immediately obtained.

## 2. Algorithm

Our algorithm is based on the randomized column selection method for low-rank matrix, recently developed in [12,28]. For an $m \times n$ matrix $A$, the column selection method looks for an interpolative decomposition to approximate $A \approx CP$ such that the discrepancy $\|A - CP\|$ is minimized, where $C$ is an $m \times c$ matrix consists of $c$ columns of $A$ and $P$ is a $c \times n$ matrix. The interpolative decomposition based on randomized column selection has recently been used for finding