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# An Extension of the COCR Method to Solving Shifted Linear Systems with Complex Symmetric Matrices

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**Abstract.** The Conjugate Orthogonal Conjugate Residual (COCR) method [T. Sogabe and S.-L. Zhang, JCAM, 199 (2007), pp. 297-303.] has recently been proposed for solving complex symmetric linear systems. In the present paper, we develop a variant of the COCR method that allows the efficient solution of complex symmetric shifted linear systems. Some numerical examples arising from large-scale electronic structure calculations are presented to illustrate the performance of the variant.

**Key words**: Shifted linear systems, complex symmetric matrices, COCR, Krylov subspace methods, electronic structure calculation.

## 1. Introduction

We consider the solution of shifted linear systems of the form:

$$A(\sigma_k)\boldsymbol{x}^{(k)} = \boldsymbol{b} \quad \text{for all } k \in S := \{1, 2, \cdots, m\}, \tag{1.1}$$

where $A(\sigma_k) := A + \sigma_k I \in \mathbb{C}^{N\times N}$ is not Hermitian but a complex symmetric sparse matrix, i.e. $A(\sigma_k) = A(\sigma_k)^T \neq \bar{A}(\sigma_k)^T$, with a scalar shift $\sigma_k \in \mathbb{C}$, and $\boldsymbol{x}^{(k)}, \boldsymbol{b}$ are complex vectors of length $N$. The shifted linear systems arise in large-scale electronic structure calculations [15] and there is a strong need for a fast solution method.

For solving (1.1), Krylov subspace methods are very attractive, since the coefficient matrices are sparse. Moreover, in this case we can use the well-known *shift-invariance property of Krylov subspaces*:

$$K_n(A(\sigma_i), \boldsymbol{b}) = K_n(A(\sigma_j), \boldsymbol{b}), \quad 1 \le i, j \le m, \tag{1.2}$$

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where $K_n(A, \boldsymbol{b}) := \text{span}\{\boldsymbol{b}, A\boldsymbol{b}, \cdots, A^{n-1}\boldsymbol{b}\}$. The latter property means that only one Krylov subspace for solving $m$ linear systems must be generated. So, when one finds approximate solutions over Krylov subspaces, one can save the costs of generating $m-1$ Krylov subspaces. This approach was shown to be highly effective: cf. [1, 6] for Hermitian positive definite case; [4, 5] for non-Hermitian case; and [3, 13, 15] for complex symmetric case (1.1).

For solving (1.1), the shifted COCG method [15] and the shifted QMR-type methods [3, 13] are powerful solvers. They are based on the shift invariance property (1.2) and basic solvers for complex symmetric linear systems, i.e. the COCG method [16] and the QMR method [3]. Although these methods are powerful, they fall into one group that uses the complex symmetric Lanczos process - e.g. see, [2, Algorithm 2.1]. This means that if the shifted QMR-type methods fail, the shifted COCG method may also fail, and vice versa. So, it is still worth finding an algorithm that is based on a different principle, in order to reduce the risk of facing such a situation in practice. The purpose of this paper is to find an algorithm using a different principle from the complex symmetric Lanczos process, as efficient as the shifted COCG method and the shifted QMR-type methods. In this paper, we consider the COCR method [12] that is based on $A$-conjugate orthogonalization process for solving complex symmetric linear systems, and then we develop the COCR method in order to solve the shifted linear systems (1.1).

The rest of this paper is organized as follows: in the next section, we review the algorithm of COCR and its main property. In Section 3, we develop a numerical method named Shifted COCR, in order to solve complex symmetric shifted linear systems, and describe the algorithm in a complete form. In Section 4, we report the results of some numerical examples. Finally, we make some concluding remarks in Section 5.

## 2. The COCR Method

In this Section, we briefly review the COCR method [12]. The COCR method is a Krylov subspace method for solving complex symmetric linear systems, and it is derived from a $A$-conjugate orthogonalization process (that is a special case of $A$-biorthogonalization process [11]) of Krylov subspace. Here we describe below the algorithm of COCR when applied to the system $A\boldsymbol{x} = \boldsymbol{b}$ with a complex symmetric matrix $A$.

Observing Algorithm 1, the $n$th residual vector can be written as

$$\boldsymbol{r}_n := \boldsymbol{b} - A\boldsymbol{x}_n = R_n(A)\boldsymbol{r}_0, \tag{2.1}$$

where the polynomial $R_n(\lambda)$ with a scalar $\lambda$ is written by the following coupled two-term recurrence relation:

$$\begin{aligned} R_0(\lambda) &= 1, \quad P_0(\lambda) = 1, \\ R_n(\lambda) &= R_{n-1}(\lambda) - \alpha_{n-1}\lambda P_{n-1}(\lambda), \\ P_n(\lambda) &= R_n(\lambda) + \beta_{n-1}P_{n-1}(\lambda), \quad n = 1, 2, \cdots, \end{aligned}$$