

## POLYNOMIAL PRECONDITIONING FOR THE GENERANK PROBLEM\*

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**Abstract.** Identifying key genes involved in a particular disease is a very important problem in biomedical research. The GeneRank model is based on the PageRank algorithm and shares many of its mathematical properties. The model brings together gene expression information with a network structure and ranks genes based on the results of microarray experiments combined with gene expression information, for example, from gene annotations (GO). In this study, we present a polynomial preconditioned conjugate gradient algorithm to solve the GeneRank problem and study its properties. Some numerical experiments are given to show the effectiveness of the suggested preconditioner.

**Key words.** gene network, gene ontologies, conjugate gradient, Chebyshev polynomial, preconditioner, M-matrix

**AMS subject classifications.** 65F10, 65F50, 9208, 92D20

**1. Introduction.** Identifying genes involved in a particular disease is regarded as a great challenge in post-genome medical research. Such identification can provide us with a better understanding of the disease. Furthermore, it is often considered as the first step in finding treatments. However, the genetic bases of many multifactorial diseases are still uncertain, and modern technologies usually report hundreds or thousands of genes related to a disease of interest. In this context, gene-disease prioritization methods are of use.

The act of finding the most potentially successful genes among a variety of listed genes has been defined as the gene prioritization problem. Considering the rapid growth in biological data sources containing gene-related information such as, for instance, sequence information, microarray expression data, functional annotation data, protein-protein interaction data, and the biological and medical literature, we can observe much interest in recent years in developing bioinformatics approaches that can analyze these data and help with the identification of important genes. The common aim in the present study is to prioritize the genes in a way that those related to the disease under study possibly appear at the top of a ranking.

In the last decade, several methods have been proposed for ranking or prioritizing genes by relevance to a disease. Some of these methods have been collected at the Gene Prioritization Portal<sup>1</sup>. These methods fall into two broad classes. The first class of methods mostly uses microarray expression data; these methods focus on identifying genes that are differentially expressed in a disease and use simple statistical measures such as the  $t$ -statistic or related classification methods in machine learning to rank genes based on this property. The second class of methods is often more general making use of a variety of data sources; these methods start with some existing knowledge of ‘training’ genes already known to be related to the disease under study and directly or indirectly rank the remaining genes based on their similarity to these training genes. There are also some methods that rank or prioritize genes based on their overall likelihood of being involved in some disease in general.

Those kinds of methods that aim to improve an initial ranking obtained from expression data by augmenting it with a network structure derived from other data sources can be related to the methods of the second class. For example, the GeneRank algorithm of Morrison et al. [8] is an intuitive modification of the PageRank algorithm used by the Google search engine that preserves many of its mathematical properties. It combines gene expres-

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<sup>1</sup><http://homes.esat.kuleuven.be/~bioiuser/gpp/index.php>

sion information with a network structure derived from gene annotations (gene ontologies (GO)) or expression profile correlations. In the resulting gene ranking algorithm, the ranking of genes can be obtained by solving a large linear system of equations. Wu et al. [10, 11] have shown that it is equivalent to a symmetric positive definite linear system of equations and have analyzed its properties. They use the conjugate gradient (CG) algorithm (see [7, 9]) in conjunction with a diagonal scaling to solve the corresponding system. Recently, Benzi and Kuhlemann in [4] have shown that the GeneRank problem system is equivalent to linear equations where the coefficient matrices are M-matrices. They have implemented the Chebyshev iteration method and methods based on polynomials of best approximation to solve the system. Their numerical experiments indicate that Chebyshev acceleration is the most effective one among the tested methods in terms of solution times. In this paper, we propose a polynomial preconditioner for the GeneRank problem and study its properties.

Throughout this paper, we use the following notations, definitions, and results. A matrix  $A$  is called nonnegative (positive) and is denoted by  $A \geq 0$  ( $A > 0$ ) if each entry of  $A$  is nonnegative (positive). Similarly, for  $n$ -dimensional vectors, by identifying them with  $n \times 1$  matrices, we can also define  $x \geq 0$  and  $x > 0$ . For a square matrix  $A$ , an eigenvalue of  $A$  is denoted by  $\lambda(A)$  and the smallest and largest eigenvalues of  $A$  are given by  $\lambda_{\min}(A)$  and  $\lambda_{\max}(A)$ , respectively. For any symmetric positive definite matrix  $A$ , we have  $\text{Cond}(A) = \|A\|_2 \|A^{-1}\|_2 = \lambda_{\max}(A)/\lambda_{\min}(A)$ ; see [2].

**DEFINITION 1.1** (see [5]). *A matrix  $A = (a_{ij}) \in \mathbb{R}^{n \times n}$  is called a nonsingular M-matrix if it can be expressed in the form  $A = rI - B$  where  $r > 0$  and  $B$  is nonnegative with spectral radius  $\rho(B) < r$ .*

The rest of the paper is organized as follows. In Section 2 we introduce the GeneRank problem in detail. Section 3 is devoted to the description of the proposed preconditioner. In Section 4 we present some numerical experiments to show the effectiveness of the preconditioner. Finally, concluding remarks are given in Section 5.

**2. The GeneRank problem formulation.** Let the set  $G = \{g_1, \dots, g_n\}$  represent  $n$  genes in a microarray. Similar to the idea of PageRank, if a gene is connected with many highly ranked genes, it should be highly ranked as well even if it may have a low rank according to the experimental data. In GO, if two genes share at least one annotation with other genes, they are defined to be connected. From this idea, we can build a gene network, whose adjacency matrix is  $W$  with entries

$$W_{ij} = \begin{cases} 1 & \text{if } g_i \text{ and } g_j \text{ (} i \neq j \text{) have the same annotation in GO,} \\ 0 & \text{otherwise.} \end{cases}$$

In contrast to PageRank, the connections are not directed. Thus, instead of a nonsymmetric hyperlink matrix, GeneRank employs a symmetric adjacency matrix  $W$  of the gene network, i.e.,  $W^T = W$ . Let

$$\text{deg}_i = \sum_{j=1}^n w_{ij}.$$

Note that since a gene might not be connected to any of the other genes,  $W$  may have zero rows. Now, let the diagonal matrix  $D$  be defined by  $D = \text{diag}(d_1, \dots, d_n)$ , where

$$d_i = \begin{cases} \text{deg}_i & \text{if } \text{deg}_i > 0, \\ 1 & \text{otherwise.} \end{cases}$$

Then the GeneRank problem can be written as the following large scale nonsymmetric linear system (cf. Morrison et al. [8])

$$(2.1) \quad (I - \alpha W D^{-1})x = (1 - \alpha)ex,$$

where  $I$  denotes the  $n \times n$  identity matrix. Also,  $\alpha$  is a damping factor with  $0 < \alpha < 1$ , and  $ex = [ex_1, ex_2, \dots, ex_n]^T$  with  $ex_i \geq 0$  is the absolute value of the expression change for  $g_i$ ,  $i = 1, 2, \dots, n$ . The solution vector  $x$  is called the GeneRank vector, and its entries provide information about the significance of a gene. Morrison et al. suggest using  $\alpha = 0.5$ . However, the optimal choice of  $\alpha$  is still an interesting topic and deserves further studies.

Note that  $W$  is an extremely sparse matrix in general. For the computation of the GeneRank vector, Morrison et al. [8] use the Jacobi iteration to solve (2.1), which is inefficient when the problem size is very large or  $\alpha$  is very close to 1. Yue et al. [12] reformulate the GeneRank model as a linear combination of three parts and present an explicit formulation for the GeneRank vector. In Wu et al. [11], the GeneRank problem is rewritten as a large scale eigenvalue problem and solved by Arnoldi-type algorithms. In [10], Wu and coworkers have observed that the matrix  $D - \alpha W$  is a symmetric positive definite matrix and they show that the nonsymmetric linear system (2.1) can be rewritten as the following symmetric positive definite (SPD) linear system

$$(2.2) \quad (D - \alpha W)\hat{x} = (1 - \alpha)ex,$$

with  $\hat{x} = D^{-1}x$ . Note that equation (2.2) is equivalent to (2.1). With this modification, methods that are suitable for symmetric systems can be used for the GeneRank problem. In [10], a Jacobi preconditioner (symmetric diagonal scaling) on  $D - \alpha W$  is implemented. In this case, the preconditioned system is given by

$$(2.3) \quad (I - \alpha D^{-\frac{1}{2}} W D^{-\frac{1}{2}})\bar{x} = (1 - \alpha)D^{-\frac{1}{2}}ex,$$

with  $\bar{x} = D^{\frac{1}{2}}\hat{x} = D^{\frac{1}{2}}(D^{-1}x) = D^{-\frac{1}{2}}x$ .

In [10], it is also shown that the eigenvalues of the preconditioned matrix are bounded as follows:

$$(2.4) \quad \lambda_{\max}(I - \alpha D^{-\frac{1}{2}} W D^{-\frac{1}{2}}) \leq 1 + \alpha,$$

$$(2.5) \quad \lambda_{\min}(I - \alpha D^{-\frac{1}{2}} W D^{-\frac{1}{2}}) \geq 1 - \alpha.$$

These bounds are independent of the size of the matrix, and they only depend on the value of the parameter  $\alpha$  used in the GeneRank model. It is noted that Benzi and Kuhleemann [4] showed that if  $\deg_i > 0$  for all  $i$ , then the inequality in (2.5) becomes an equality; see also Lemma 3.2 below.

As mentioned above, Benzi and Kuhleemann [4] proved that the coefficient matrices of (2.1) and (2.2) have a nice property that we introduce here.

**THEOREM 2.1.** *Both of the matrices  $D - \alpha W$  and  $I - \alpha D^{-\frac{1}{2}} W D^{-\frac{1}{2}}$  are  $M$ -matrices for  $0 < \alpha < 1$ .*

In [4], the classical Chebyshev iteration for the GeneRank problem is implemented. It is a polynomial scheme to expedite the convergence of the stationary iterative method

$$x^{(k+1)} = x^{(k)} + M^{-1}(b - Ax^k), \quad k = 0, 1, \dots,$$

to solve a linear system of equation  $Ax = b$  in which  $M$  is a nonsingular matrix. If the matrix  $I - M^{-1}A$  is similar to a symmetric matrix with eigenvalues lying in an interval  $[l_{\min}, l_{\max}]$  on the positive real axis, then the Chebyshev iteration for the system  $Ax = b$

is given by (for more details, see [4, 6])

$$y^{(k+1)} = \frac{\omega_{k+1}}{2 - (l_{\min} + l_{\max})} \left\{ 2M^{-1}(b - Ay^{(k)}) + [2 - (l_{\min} + l_{\max})](y^{(k)} - y^{(k-1)}) \right\} + y^{(k-1)}, \quad k = 1, 2, \dots,$$

where  $y^{(0)} = x^{(0)}$ ,  $y^{(1)} = x^{(1)}$ , and

$$\omega_{k+1} = \frac{1}{1 - \frac{\omega_k^2}{4\omega^2}}, \quad \omega_2 = \frac{2\omega^2}{2\omega^2 - 1}, \quad \omega_1 = 1, \quad \omega = \frac{2 - (l_{\min} + l_{\max})}{l_{\max} - l_{\min}}.$$

For the GeneRank problem, the setting  $l_{\min} = 1 - \alpha$ ,  $l_{\max} = 1 + \alpha$ ,  $A = D - \alpha W$ ,  $b = ex$ , and  $M = D = \text{diag}(A)$  is used.

Numerical results presented in [4] show that the number of iterations of this method is usually higher than those of the CG method with diagonal scaling. However, the cost per iteration is much lower, and this leads to faster convergence in terms of CPU time.

**3. Main results.** Wu et al. [10, 11] proved that the coefficient matrix of (2.2) is symmetric positive definite, and therefore the CG method can be used to solve the system. As it is well-known, the convergence rate of the CG method depends on the condition number of the matrix in question or more generally on the distribution of the eigenvalues. If the eigenvalue distribution of the preconditioned system is more clustered than that of the original one, the convergence will be accelerated drastically. Having this in mind, Wu et al. apply the Jacobi preconditioner to the system (2.2) to accelerate the convergence rate of the method. In this case, the linear system (2.3) is obtained. Considering (2.4) and (2.5), we can conclude that increasing  $\alpha$  from 0 to 1 can cause an increase in the ratio  $\lambda_{\max}/\lambda_{\min}$ , and therefore the coefficient matrix would be increasingly ill-conditioned, and the rate of convergence of CG is expected to decrease as  $\alpha$  increases.

From now on, for the sake of the simplicity, let  $J_\alpha = \alpha D^{-\frac{1}{2}} W D^{-\frac{1}{2}}$  and  $S_\alpha = I - J_\alpha$ . It is noted that the matrix  $S_\alpha$  is the coefficient matrix of the system (2.3). We now propose the preconditioner  $M_\alpha = I + J_\alpha$  for the system (2.3). In this case, the preconditioned system takes the form

$$M_\alpha S_\alpha \bar{x} = M_\alpha b_\alpha,$$

where  $b_\alpha = (1 - \alpha)D^{-\frac{1}{2}}ex$ . In the following, we investigate the properties of the proposed preconditioner.

**THEOREM 3.1.** *For every  $0 < \alpha < 1$ , the matrix  $M_\alpha S_\alpha$  is a symmetric positive definite M-matrix.*

*Proof.* Since the matrix  $D^{-\frac{1}{2}} W D^{-\frac{1}{2}}$  is sub-stochastic (nonnegative with row sums less than or equal to 1), we have  $\rho(J_\alpha) \leq \alpha < 1$ . Hence  $\rho(J_\alpha^2) \leq \alpha^2 < 1$ , and since  $J_\alpha$  is nonnegative, it follows from Definition 1.1 that the matrix  $T_\alpha = I - J_\alpha$  is an M-matrix.  $\square$

**LEMMA 3.2.** *If  $W \neq 0$ , then  $\lambda_{\min}(S_\alpha) = 1 - \alpha$ .*

*Proof.* Let  $x = (x_1, \dots, x_n)^T$  such that

$$x_i = \begin{cases} 1 & \text{if } \deg_i > 0, \\ 0 & \text{otherwise,} \end{cases}$$

for  $i = 1, 2, \dots, n$ . Obviously, we have  $Wx = Dx$ . Now, observing that  $y = D^{\frac{1}{2}}x \neq 0$ , we get

$$(I - \alpha D^{-\frac{1}{2}}WD^{-\frac{1}{2}})y = (1 - \alpha)y,$$

which is equivalent to  $S_\alpha y = (1 - \alpha)y$ . By equation (2.5), we obtain that  $1 - \alpha$  is the smallest eigenvalue of  $S_\alpha$ .  $\square$

REMARK 3.3. In [10] it has been shown that

$$(3.1) \quad \lambda_{\max}(WD^{-1}) \leq 1, \quad \lambda_{\min}(WD^{-1}) \geq -1.$$

Since the eigenvalues of  $D^{-\frac{1}{2}}WD^{-\frac{1}{2}}$  are the same as those of  $WD^{-1}$ , we deduce from equation (3.1) and Lemma 3.2 that

$$(3.2) \quad \lambda_{\max}(I - J_\alpha^2) \leq 1 + \alpha^2, \quad \text{and} \quad \lambda_{\min}(I - J_\alpha^2) = 1 - \alpha^2.$$

THEOREM 3.4. *The spectral condition number of  $T_\alpha$  is not greater than that of the matrix  $S_\alpha$ , i.e.,*

$$\text{Cond}_2(T_\alpha) \leq \text{Cond}_2(S_\alpha).$$

*Proof.* Since both of the matrices  $S_\alpha$  and  $T_\alpha$  are symmetric positive definite, it is enough to prove that

$$\frac{\lambda_{\max}(T_\alpha)}{\lambda_{\min}(T_\alpha)} \leq \frac{\lambda_{\max}(S_\alpha)}{\lambda_{\min}(S_\alpha)}.$$

For every eigenvalue  $\lambda(S_\alpha)$  of  $S_\alpha$ , we have  $\lambda_{\min}(S_\alpha) \leq \lambda(S_\alpha) \leq \lambda_{\max}(S_\alpha)$ . Then,

$$1 - \lambda_{\max}(S_\alpha) \leq 1 - \lambda(S_\alpha) \leq 1 - \lambda_{\min}(S_\alpha).$$

From Lemma 3.2, we have  $\lambda_{\min}(S_\alpha) \leq 1$ . We now consider two cases,  $\lambda_{\max}(S_\alpha) \geq 1$  and  $\lambda_{\max}(S_\alpha) < 1$ . If  $\lambda_{\max}(S_\alpha) \geq 1$ , then by equation (2.4) and Lemma 3.2, we have the upper bound  $\lambda_{\max}(S_\alpha) - 1 \leq 1 - \lambda_{\min}(S_\alpha)$ . Therefore  $1 - (1 - \lambda_{\max}(S_\alpha))^2 \geq 1 - (1 - \lambda_{\min}(S_\alpha))^2$ , and since the maximum value of  $1 - (1 - \lambda(S_\alpha))^2$  is equal to 1, we obtain

$$\text{Cond}(T_\alpha) \leq \frac{1}{1 - (1 - \lambda_{\min}(S_\alpha))^2} \leq \frac{\lambda_{\max}(S_\alpha)}{\lambda_{\min}(S_\alpha)} = \text{Cond}(S_\alpha).$$

Now, suppose that  $\lambda_{\max}(S_\alpha) \leq 1$ . In this case, it is easy to see that

$$\text{Cond}(T_\alpha) = \frac{1 - (1 - \lambda_{\max}(S_\alpha))^2}{1 - (1 - \lambda_{\min}(S_\alpha))^2} \leq \frac{\lambda_{\max}(S_\alpha)}{\lambda_{\min}(S_\alpha)} = \text{Cond}(S_\alpha).$$

Thus, the proof is completed.  $\square$

This theorem shows that the eigenvalues of the matrix  $T_\alpha$  are clustered at least as much as those of the matrix  $S_\alpha$ . As we shall see, for the presented numerical experiments, the eigenvalues of  $T_\alpha$  are more clustered than those of  $S_\alpha$ .

REMARK 3.5. From Lemma 3.2, if  $W \neq 0$ , then  $\lambda_{\min}(S_\alpha) = 1 - \alpha$ . Therefore, according to the relation  $\lambda(T_\alpha) = 1 - (1 - \lambda(S_\alpha))^2$ , we have  $\lambda_{\min}(T_\alpha) = 1 - \alpha^2$ . Having in mind that  $0 < \lambda(T_\alpha) < 1$ , we deduce that  $1 - \alpha^2 \leq \lambda(T_\alpha) < 1$ . Note that  $1 - \alpha \leq \lambda(S_\alpha) \leq 1 + \alpha$ .

We remark that the matrix  $M_\alpha$  is the first degree polynomial preconditioner obtained by truncating the Neumann series expansion of  $S_\alpha^{-1}$  to first order:

$$(3.3) \quad S_\alpha^{-1} = (I - J_\alpha)^{-1} = I + J_\alpha + J_\alpha^2 + \cdots \approx I + J_\alpha \equiv M_\alpha.$$

Some other properties of such a preconditioner can be found in [1, 9]. One may obtain similar preconditioners by using higher degree polynomial approximations in (3.3). Hereafter, we set  $\bar{M}_\alpha = I + J_\alpha + J_\alpha^2$  and  $\tilde{M}_\alpha = I + J_\alpha + J_\alpha^2 + J_\alpha^3$ .

**4. Numerical experiments.** As mentioned above, in [10] the Jacobi preconditioner in conjunction with the CG algorithm is successfully applied to the solution of the linear system and it is deduced that it is the fastest among the tested methods for each of the presented examples. Also, Benzi and Kuhlemann in [4] compare the Chebyshev method and the method based on polynomials of best approximation with a CG method and a Jacobi-preconditioned CG method, and they show that in conjunction with diagonal scaling, Chebyshev acceleration can significantly outperform CG in terms of solution times.

In this section we compare the numerical results of CG and the Chebyshev iteration methods with the first and third degree polynomial preconditioners to those of the Jacobi preconditioner and Chebyshev acceleration. With attention to (3.2), we consider the first degree polynomial preconditioner of the Chebyshev iteration with the setting  $l_{\min} = 1 - \alpha^2$ ,  $l_{\max} = 1 + \alpha^2$ ,  $A = D - \alpha W$ ,  $b = ex$ , and  $M = D = \text{diag}(A)$ .

All the numerical experiments presented in this section are computed in double precision and the algorithms are implemented in MATLAB 7.12.0 and tested on a 64-bit 1.73 GHz intel Q740 core i7 processor with 4GB RAM running Windows 7. We use a stopping criteria based on the 1-norm of the residual. That is, we stop iterating as soon as  $\|r\|_1 < tol$ , where  $tol$  is a given tolerance. The initial guess is the null vector. We use two different choices for  $ex$ ,  $ex = (\frac{1}{n})e$ , where  $e$  is the vector of all ones, and  $ex = p$ , where  $p$  is a randomly chosen probability vector, that is, a random vector with entries in  $(0, 1)$ . For each adjacency matrix, we use four different values of  $\alpha$  to form the corresponding GeneRank matrices  $D - \alpha W$ ,  $\alpha = 0.5, 0.75, 0.80, 0.99$ . The obtained numerical results are presented in the tables below. In all the tables, “CG”, “PCG”, “Chebyshev”, “Chebyshev- $M_\alpha$ ”, “CG- $M_\alpha$ ”, and “CG- $\tilde{M}_\alpha$ ” denote, respectively, the CG method implemented for the system (2.2), the CG method applied to the system (2.3), the Chebyshev iteration for (2.2), the preconditioned Chebyshev iteration for the system (2.2) with the preconditioner  $M_\alpha$ , and the CG algorithm for the system (2.2) in conjunction with the preconditioners  $M_\alpha$ ,  $\bar{M}_\alpha$ , and  $\tilde{M}_\alpha$ .

**EXAMPLE 4.1.** In this example three adjacency matrices are used,  $w\_All$ , which is of size  $4047 \times 4047$  with 339596 nonzero entries,  $w\_Up$ , which is of size  $2392 \times 2392$  with 128468 nonzero entries, and  $w\_Down$ , which is of size  $1625 \times 1625$  with 67252 nonzero entries, and three expression change vectors  $expr\_data$ ,  $expr\_dataUp$ , and  $expr\_dataDown$ . These matrices were constructed using all the three sections of the GO, where a link is presented between two genes if they share a GO annotation. Only genes which are up-regulated are included in  $w\_Up$  and only down-regulated ones in  $w\_Down$  [8]. The data files are available from [3]. The results for these matrices are given in Tables 4.1, 4.2, and 4.3. In these tables (as for the other tables below), the number of iterations for convergence together with the CPU time in seconds (in parenthesis) are given. Here we mention that, in this example, the tolerance  $tol$  is taken to be  $10^{-14}$ . For this example, as the numerical results show, the CG method with the preconditioners  $M_\alpha$ ,  $\bar{M}_\alpha$ , and  $\tilde{M}_\alpha$  outperforms the other tested methods in terms of both the number of iterations and the CPU time. Moreover, the results are especially attractive for  $\alpha$  close to 1. We also observe that the number of iterations of the CG method with  $\tilde{M}_\alpha$  is always less than those of the CG method with the preconditioner  $M_\alpha$ , while the CPU time for the CG method with  $M_\alpha$  is less than that with the preconditioner  $\tilde{M}_\alpha$ . As Axelsson noted

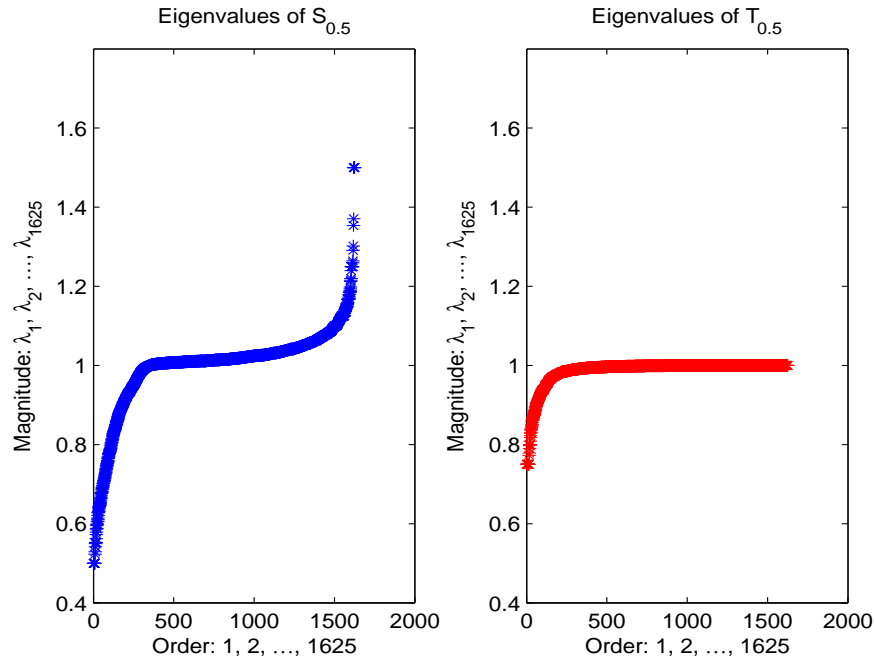


FIG. 4.1. Eigenvalue distribution of  $S_{0.5}$  and  $T_{0.5}$  for the matrix  $w\_Down$ .

in [1], using first degree polynomials roughly halves the number of CG iterations (at the price of two matrix-vector multiplications per iteration), while using third degree polynomials reduces the number of iterations roughly by a factor of three (at the price of three matrix-vector multiplications per iteration) and so on. Hence, polynomial preconditioners do not reduce the total number of matrix-vector multiplications but only the number of vector operations (linked triads, inner products, etc). This means that these methods can be effective only if the coefficient matrices are extremely sparse (as in the GeneRank problem) or, more generally, when the matrix-vector operations are very cheap. This fact can be observed when the results of CG are compared to those of  $CG-M_\alpha$  and  $CG-\tilde{M}_\alpha$ . The last comment here is that the number of iterations of the  $CG-\tilde{M}_\alpha$  method is slightly smaller than that of  $CG-M_\alpha$ , but the difference is not significant. Additional performed numerical experiments show that among the preconditioners of the form  $I + J_\alpha + J_\alpha^2 + \dots + J_\alpha^r$ , the ones with odd values of  $r$  are preferred over such preconditioners with even  $r$ ; see [1, p. 181].

For a further investigation, in Figures 4.1, 4.2, and 4.3, we depict the eigenvalues distribution of  $S_\alpha$  and  $T_\alpha$  for the test matrices  $w\_Down$  when  $\alpha = 0.5$ ,  $w\_Up$  when  $\alpha = 0.75$ , and  $w\_All$  when  $\alpha = 0.9$ , respectively. As it can be observed, the eigenvalues of the matrices  $T_\alpha$  are more clustered than those of  $S_\alpha$  for all three test matrices.

**EXAMPLE 4.2.** In this example we use two different types of test data for our experiments. The first matrix is the SNP<sub>a</sub> adjacency matrix (single-nucleotide polymorphism matrix). This matrix has  $n = 152520$  rows and columns and is very sparse with only 639,248 nonzero entries. The second type is a RENG<sub>a</sub> adjacency matrix (range-dependent random graph model). In our experiments we set  $\lambda = 0.9$  and  $\beta = 1$ , the default values in RENG<sub>a</sub>. Both of these types of matrices are tested in [4, 10]. The results for the SNP<sub>a</sub> matrix are given in Tables 4.4 and 4.5, and the results for the RENG<sub>a</sub> matrix with  $n = 100000$  and  $n = 500000$  are given in Tables 4.6 and 4.7. In this example the tolerance  $tol$  is set to  $10^{-10}$ . All the comments made for the previous example remain valid.



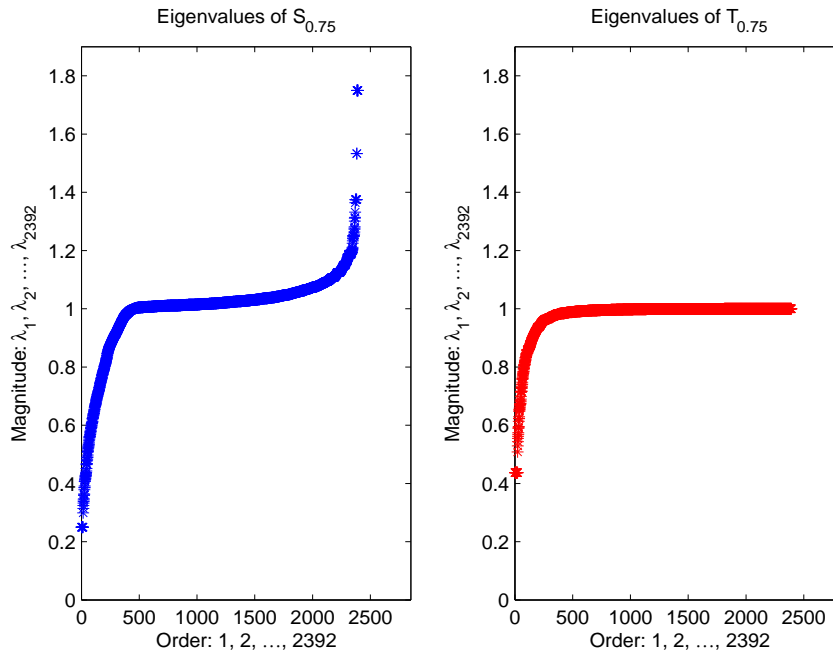


FIG. 4.2. Eigenvalue distribution of  $S_{0.75}$  and  $T_{0.75}$  for the matrix  $w_{Up}$ .

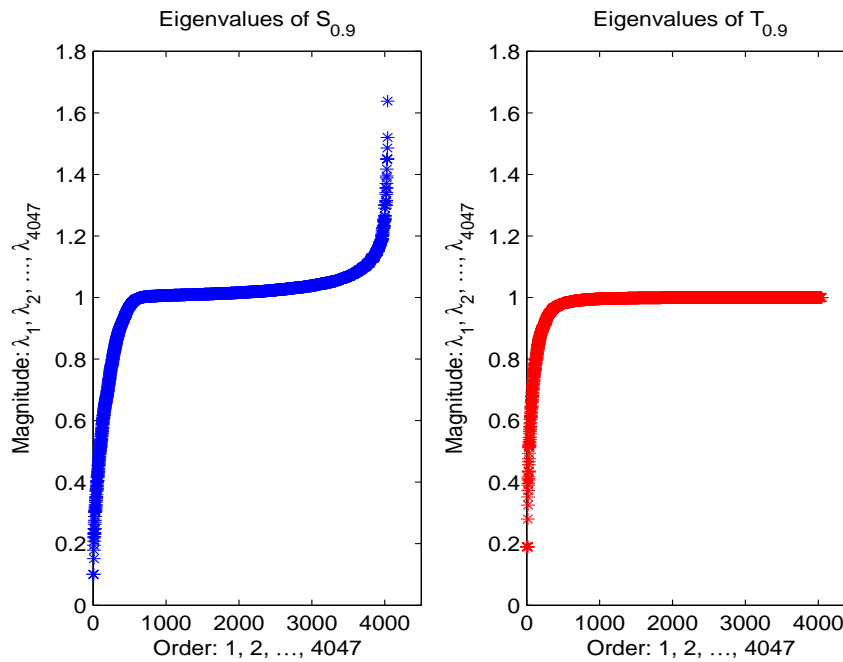


FIG. 4.3. Eigenvalue distribution of  $S_{0.9}$  and  $T_{0.9}$  for the matrix  $w_{All}$ .



TABLE 4.1  
*Results for the w\_All matrix in Example 4.1. Here  $ex = extr\_data$ .*

$\alpha$	0.50	0.75	0.80	0.99
CG	381 (0.700)	441 (0.772)	456 (0.785)	603 (1.012)
PCG	26 (0.051)	39 (0.082)	42 (0.081)	69 (0.133)
Chebyshev	23 (0.030)	36 (0.048)	41 (0.057)	177 (0.195)
Chebyshev- $M_\alpha$	15 (0.086)	25 (0.094)	28 (0.108)	126 (0.253)
Chebyshev- $\bar{M}_\alpha$	11 (0.033)	19 (0.106)	23 (0.099)	104 (0.324)
CG- $M_\alpha$	11 (0.023)	16 (0.037)	18 (0.044)	30 (0.064)
CG- $\bar{M}_\alpha$	10 (0.080)	15 (0.076)	17 (0.056)	29 (0.099)
CG- $\tilde{M}_\alpha$	7 (0.030)	11 (0.046)	13 (0.054)	22 (0.102)

TABLE 4.2  
*Results for the matrix w\_Up in Example 4.1. Here  $ex = extr\_dataUp$ .*

$\alpha$	0.50	0.75	0.80	0.99
CG	309 (0.142)	360 (0.162)	377 (0.173)	488 (0.221)
PCG	26 (0.017)	39 (0.026)	42 (0.022)	70 (0.033)
Chebyshev	22 (0.008)	36 (0.013)	41 (0.014)	177 (0.058)
Chebyshev- $M_\alpha$	15 (0.019)	25 (0.023)	28 (0.025)	127 (0.071)
Chebyshev- $\bar{M}_\alpha$	11 (0.021)	20 (0.024)	23 (0.028)	105 (0.082)
CG- $M_\alpha$	11 (0.006)	16 (0.011)	18 (0.012)	31 (0.017)
CG- $\bar{M}_\alpha$	10 (0.009)	15 (0.013)	16 (0.014)	29 (0.025)
CG- $\tilde{M}_\alpha$	7 (0.008)	11 (0.016)	13 (0.014)	22 (0.022)

TABLE 4.3  
*Results for the matrix w\_Down in Example 4.1. Here  $ex = extr\_dataDown$ .*

$\alpha$	0.50	0.75	0.80	0.99
CG	267 (0.087)	310 (0.091)	322 (0.094)	427 (0.131)
PCG	27 (0.010)	40 (0.013)	44 (0.014)	76 (0.024)
Chebyshev	22 (0.007)	35 (0.008)	40 (0.009)	173 (0.035)
Chebyshev- $M_\alpha$	14 (0.016)	24 (0.012)	28 (0.013)	125 (0.041)
Chebyshev- $\bar{M}_\alpha$	11 (0.010)	19 (0.013)	22 (0.014)	103 (0.046)
CG- $M_\alpha$	11 (0.006)	17 (0.006)	18 (0.006)	32 (0.013)
CG- $\bar{M}_\alpha$	10 (0.004)	16 (0.006)	17 (0.008)	32 (0.020)
CG- $\tilde{M}_\alpha$	7 (0.007)	12 (0.012)	13 (0.011)	23 (0.014)

TABLE 4.4  
*Results for the SNPa matrix in Example 4.2. Here  $ex = (\frac{1}{n})e$ , where  $e$  is the vector of all ones.*

$\alpha$	0.50	0.75	0.80	0.99
CG	86 (2.420)	116 (3.321)	128 (3.663)	469 (13.32)
PCG	17 (0.514)	27 (0.818)	30 (0.922)	91 (2.738)
Chebyshev	17 (0.208)	28 (0.359)	31 (0.384)	130 (1.402)
Chebyshev- $M_\alpha$	11 (0.244)	19 (0.352)	22 (0.382)	95 (1.246)
Chebyshev- $\bar{M}_\alpha$	9 (0.298)	15 (0.346)	18 (0.401)	79 (1.464)
CG- $M_\alpha$	9 (0.164)	13 (0.213)	15 (0.236)	44 (0.704)
CG- $\bar{M}_\alpha$	8 (0.163)	14 (0.287)	16 (0.342)	52 (1.086)
CG- $\tilde{M}_\alpha$	6 (0.195)	9 (0.269)	10 (0.262)	33 (0.963)

TABLE 4.5

Results for the SNPa matrix in Example 4.2. Here  $ex = p$ , where  $p$  is a random probability vector.

$\alpha$	0.50	0.75	0.80	0.99
CG	127 (3.649)	174 (5.011)	193 (5.607)	721 (20.41)
PCG	26 (0.789)	41 (1.242)	46 (1.375)	139 (4.203)
Chebyshev	17 (0.211)	27 (0.354)	30 (0.352)	125 (1.368)
Chebyshev- $M_\alpha$	11 (0.259)	19 (0.382)	21 (0.367)	92 (1.222)
Chebyshev- $\tilde{M}_\alpha$	9 (0.267)	15 (0.396)	17 (0.414)	77 (1.349)
CG- $M_\alpha$	8 (0.170)	13 (0.209)	14 (0.232)	43 (0.713)
CG- $\tilde{M}_\alpha$	8 (0.175)	14 (0.279)	16 (0.355)	51 (1.069)
CG- $\tilde{M}_\alpha$	6 (0.171)	9 (0.245)	10 (0.261)	32 (0.908)

TABLE 4.6

Results for the RENGA matrices in Example 4.2. Here  $ex = (\frac{1}{n})e$ , where  $e$  is the vector of all ones.

$n = 100000$				
$\alpha$	0.50	0.75	0.80	0.99
CG	43 (0.789)	47 (0.840)	48 (0.863)	129 (2.305)
PCG	14 (0.262)	22 (0.431)	24 (0.459)	95 (1.824)
Chebyshev	17 (0.183)	27 (0.245)	31 (0.259)	127 (0.905)
Chebyshev- $M_\alpha$	11 (0.244)	19 (0.352)	22 (0.382)	95 (1.246)
Chebyshev- $\tilde{M}_\alpha$	9 (0.238)	15 (0.331)	17 (0.358)	78 (1.083)
CG- $M_\alpha$	8 (0.092)	12 (0.141)	14 (0.168)	53 (0.673)
CG- $\tilde{M}_\alpha$	7 (0.120)	11 (0.192)	12 (0.234)	51 (0.885)
CG- $\tilde{M}_\alpha$	5 (0.118)	9 (0.201)	10 (0.226)	41 (0.935)
$n = 500000$				
CG	23 (2.612)	27 (3.006)	30 (3.398)	106 (12.02)
PCG	13 (1.578)	20 (2.453)	22 (2.661)	86 (10.50)
Chebyshev	17 (0.901)	27 (1.371)	30 (1.512)	125 (6.359)
Chebyshev- $M_\alpha$	11 (1.655)	19 (2.231)	21 (2.364)	91 (7.240)
Chebyshev- $\tilde{M}_\alpha$	8 (1.802)	15 (2.482)	17 (2.542)	76 (8.082)
CG- $M_\alpha$	5 (0.645)	12 (1.100)	14 (1.234)	50 (4.671)
CG- $\tilde{M}_\alpha$	6 (0.743)	10 (1.223)	11 (1.384)	44 (5.555)
CG- $\tilde{M}_\alpha$	5 (0.768)	8 (1.214)	9 (1.436)	38 (6.098)

**5. Conclusion.** In this paper, a simple polynomial preconditioner has been implemented and tested for the GeneRank problem, and some of its properties have been illustrated. Finally, numerical experiments have been presented to show the effectiveness of the proposed preconditioner. As it can be observed, it does not need any CPU time to set up the preconditioner and the preconditioner is explicitly at hand. Our numerical results show that the proposed preconditioner is more effective than the ones presented in the literature.

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TABLE 4.7  
*Results for the RENGA matrices in Example 4.2. Here  $\epsilon x = p$ , where  $p$  is arandom probability vector.*

$n = 100000$				
$\alpha$	0.50	0.75	0.80	0.99
CG	68 (1.254)	73 (1.299)	75 (1.337)	222 (4.021)
PCG	22 (0.418)	34 (0.667)	39 (0.732)	165 (3.286)
Chebyshev	17 (0.167)	26 (0.255)	30 (0.269)	122 (0.883)
Chebyshev- $M_\alpha$	11 (0.257)	19 (0.289)	22 (0.335)	93 (0.949)
Chebyshev- $\bar{M}_\alpha$	8 (0.237)	15 (0.306)	17 (0.335)	75 (0.998)
CG- $M_\alpha$	8 (0.093)	12 (0.145)	14 (0.170)	53 (0.668)
CG- $\bar{M}_\alpha$	7 (0.123)	11 (0.185)	12 (0.216)	51 (0.903)
CG- $\tilde{M}_\alpha$	5 (0.105)	9 (0.185)	10 (0.212)	40 (0.877)
$n = 500000$				
CG	36 (4.101)	45 (5.109)	50 (5.637)	200 (22.68)
PCG	21 (2.509)	34 (4.168)	38 (4.585)	163 (19.84)
Chebyshev	16 (0.838)	26 (1.360)	29 (1.455)	120 (6.062)
Chebyshev- $M_\alpha$	11 (1.702)	18 (2.153)	21 (2.409)	88 (6.712)
Chebyshev- $\bar{M}_\alpha$	8 (1.750)	14 (2.464)	17 (2.556)	73 (7.950)
CG- $M_\alpha$	8 (0.733)	12 (1.094)	13 (1.174)	51 (4.761)
CG- $\bar{M}_\alpha$	6 (0.807)	10 (1.244)	11 (1.391)	46 (5.854)
CG- $\tilde{M}_\alpha$	5 (0.796)	8 (0.236)	10 (1.586)	39 (6.050)

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