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A HERMITIAN LANCZOS METHOD FOR NORMAL MATRICES

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Abstract: *We derive an algorithm for solving iteratively a linear system $Nx = b$ involving a large, possibly sparse normal matrix $N \in \mathbb{C}^{n\times n}$ and a vector $b \in \mathbb{C}^n$. The introduced method is based on the Toeplitz decomposition $N = H + iK$ of N, where H and K are Hermitian matrices. Generically, N is polynomial of H and therefore, since N^{-1} is a polynomial of N, also N^{-1} is a polynomial of H. This gives rise to a Krylov scheme for solving $Nx = b$ via*

$$\min_{p_{j-1}\in\mathcal{P}_{j-1}} \|Np_{j-1}(H)b - b\| = \min_{p_{j-1}\in\mathcal{P}_{j-1}} \|p(H)_{j-1}Nb - b\|$$

as H and N commute. Consequently, at j^{th} step, we have a minimization problem that is equivalent with finding the best approximant to b from the Krylov subspace $\mathcal{K}_j(H; Nb)$. Based on this, we obtain an optimal algorithm for solving $Nx = b$ that is realizable with a 3-term recurrence.

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1 Introduction

The set of normal matrices, denoted by $\mathcal{N} \subset \mathbb{C}^{n\times n}$, is a rich class of matrices well-suited for numerical computations. To give an example of the computational well-behavior, extreme sensitivity of eigenvalues and eigenvectors does not occur among the set of normal matrices. In the domain of algorithms, a lot of methods exists exclusively for a subset of $\mathcal{N}$, namely for Hermitian matrices. However, for non-Hermitian *normal* matrices typically no specific schemes have been developed. Then problems are solved by executing more general algorithms that benefit in no way from normality which can be considered to be a severe waste of available structure. In this paper we introduce an optimal Krylov method especially designed for solving, with a given $b \in \mathbb{C}^n$, a linear system

$$Nx = b, \tag{1}$$

for a large, possibly sparse, invertible normal matrix N.

For solving (1) we extend the Hermitian Lanczos method to apply to normal matrices. The introduced scheme is a genuine extension as it will reduce to the Hermitian Lanczos iteration in case N is Hermitian. To this end we use the Toeplitz decomposition

$$N = H + iK, \tag{2}$$

with Hermitian $H = \frac{1}{2}(N + N^*)$ and $K = \frac{1}{2i}(N - N^*)$, of N. For normal matrices the Toeplitz decomposition has the property that, denoting by $\mathcal{H}_0$ the set of nonderogatory Hermitian matrices, the mapping

$$(H, \alpha_0, ..., \alpha_{n-1}) \to H + i\sum_{j=0}^{n-1} \alpha_j H^j \tag{3}$$

maps $\mathcal{H}_0 \times \mathbb{R}^n$ into $\mathcal{N}$. And in such a way that its image is an open dense subset of $\mathcal{N}$. Consequently, a generic normal matrix N equals $H + ip(H)$, where $H = \frac{1}{2}(N + N^*)$ and p is a polynomial with real coefficients. This holds also for normal matrices having degoratory Hermitian part under a moderate technical assumption, see Proposition 3.

As N is invertible in (1), by elementary linear algebra, its inverse is a polynomial of N. Since N is, generically, a polynomial of its Hermitian part H, we can deduce that N^{-1} is generically a polynomial of H. As a consequence, denoting by $\mathcal{P}_{j-1}$ the set of polynomials of degree $j-1$ at most, we can replace the GMRES [18] minimization problem at the j^{th} step

$$\min_{p_{j-1}\in\mathcal{P}_{j-1}} \|Np_{j-1}(N)b - b\| \tag{4}$$

with

$$\min_{p_{j-1}\in\mathcal{P}_{j-1}} \|Np_{j-1}(H)b - b\|. \tag{5}$$

Remark that the success of GMRES, in fact, relies on the simple property that the inverse of a matrix is a polynomial of the matrix itself. In practise the inverse is being approximated by *very* low degree polynomials via computing (4). The reason for this is that with GMRES the lenght of recurrencies as well as memory requirements grow linearly for non-Hermitian matrices.

To avoid long recurrencies and linear growth of memory demands we do not construct a Krylov subspace with N. Instead, since N and H commute, we derive an algorithm for solving (1) starting from (5) by considering first

$$\min_{p_{j-1}\in\mathcal{P}_{j-1}} \|p_{j-1}(H)Nb - b\|. \tag{6}$$

From this it is readily seen that solving (5) is equivalent to finding the best approximant to b from the Krylov subspace

$$\mathcal{K}_j(H; Nb) = \mathrm{span}\{Nb, HNb, ..., H^{j-1}Nb\}. \tag{7}$$

To this end one could, straightforwardly, execute the Hermitian Lanczos method with H starting from $q_0 = \frac{Nb}{\|Nb\|}$. This would yield the value of (6) and thereby of (5) with a 3-term recurrence and in such a way that only 3 vectors needed to be saved. But this scheme would not, as such, yield a solution candidate to (1) unless we multiply once by N^{-1}. This is obviously not what we suggest as the inverse of N is not available. Instead, we construct from this Hermitian Lanczos iteration a new recurrence by formally multiplying by N^{-1}. As a result, we obtain a 3-term recurrence for solving (1) with the same memory requirements as in the standard Hermitian Lanczos method. The constructed solution candidate fulfills, at each step j, the optimality condition (5) so that, whenever N is Hermitian, the introduced scheme is simply GMRES. Thus, in a sense, we extend GMRES for Hermitian matrices to normal matrices in a way that preserves an optimal 3-term recurrence property.

In addition to the obtained basic algorithm, there is a restarted and rotated implementation aimed for a nongeneric or nearly nongeneric N. This means restarting the algorithm using rotations $e^{i\theta}N$ of N for $\theta \in [0, 2\pi)$. Rotations can be chosen based on some a priori information, or they can be generated randomly after a number of steps. This can speed up convergence dramatically and, in particular, it is simple to code to increase adaptivity in the basic algorithm. We illustrate this with numerical examples.

The paper is organized as follows. In Section 2 we consider properties of the Toeplitz decomposition for normal matrices. Based on these properties we derive a minimization problem analogous to ideal GMRES. In Section 3 we consider the local version of this minization problem. This gives rise to a Hermitian Lanczos method for solving linear systems involving normal matrices. Finally in Section 4 we consider numerical experiments.

2 On the Toeplitz decomposition of a normal matrix

The set of normal matrices is a large class of matrices containing, for instance, the set of Hermitian, skew-Hermitian as well as the set of unitary matrices. For numerical manipulations normal matrices are particularly well-suited as a matrix is normal if and only if it is unitary similar to a diagonal matrix. Although this is how normality is most often used in practise, its original definition is purely algebraic in the sense that $N \in \mathbb{C}^{n\times n}$ is normal if

$$NN^* - N^*N = 0 \tag{8}$$

holds. Besides these two chracterizations, there are many ways to define normality. So far about ninety equivalent conditions for a matrix to be normal have been collected by Grone, Johnson, Sa and Wolkowicz [9] and by Elsner and Ikramov [2]. The characterization (8) is taken to be the first in these listings although it is numbered as the condition zero.

Due to the abundance of characterizations of normality, several of them deal with the canonical decompositions for matrices. Diagonalizability by a unitary similarity is, for instance, one such. Another is based on the Toeplitz decomposition

$$N = H + iK, \tag{9}$$

with $H = \frac{1}{2}(N + N^*)$ and $K = \frac{1}{2i}(N - N^*)$, of N. The condition 21 in [9] states that N is normal if and only if H and K commute. In what follows, we consider the Toeplitz decomposition for normal matrices in more detail.

First of all, commutativity is a strong property. In particular, it is well-known that for a nonderogatory matrix $A \in \mathbb{C}^{n\times n}$ the set of matrices commuting with A equals the set of polynomials of A [10]. For normal matrices this can be used as follows, where $\mathcal{N}_0$ denotes the set of normal matrices N having nonderogatory Hermitian part $H = \frac{1}{2}(N + N^*)$. In our claims regarding normal matrices we use the induced topology of the standard metric topology of $\mathbb{C}^{n\times n}$.

Theorem 1 *[12] $\mathcal{N}_0$ is an open dense subset of $\mathcal{N}$.*

This set is readily realizable. Namely, if we denote by $\mathcal{H}_0$ the set of nonderogatory Hermitian matrices, then the mapping

$$(H, \alpha_0, ..., \alpha_{n-1}) \to H + i\sum_{j=0}^{n-1} \alpha_j H^j \tag{10}$$

from $\mathcal{H}_0 \times \mathbb{R}^n$ onto $\mathcal{N}_0$ is injective. In particular, combining this with Theorem 1, we can deduce that a generic normal matrix N is a polynomial of its Hermitian part H. By a generic property in a set S we mean that it holds for an open dense subset of S. This is also true for certain matrices not belonging to $\mathcal{N}_0$. By $\sigma(A)$ we denote the spectrum of $A \in \mathbb{C}^{n\times n}$.

Theorem 2 *Assume $N = H + iK$ is normal such that $\#\sigma(N) = \#\sigma(H)$. Then $N = H + ip(H)$ for a polynomial p of degree $\#\sigma(N) - 1$ at most.*

Proof. Let N be diagonalized by a unitary matrix U so that its Toeplitz decomposition is

$$N = U \begin{bmatrix} \Re(\lambda_1) & & \\ & \ddots & \\ & & \Re(\lambda_n) \end{bmatrix} U^* + iU \begin{bmatrix} \Im(\lambda_1) & & \\ & \ddots & \\ & & \Im(\lambda_n) \end{bmatrix} U^* = H + iK, \tag{11}$$

where $\lambda_1, ...\lambda_n$ denote the eigenvalues of N, counting multiplicities, arranged in nondecreasing order of modulus. Since $\#\sigma(N) = \#\sigma(H)$, we can construct the Lagrange's interpolation polynomial p attaining the values $\Im(\lambda_1), ..., \Im(\lambda_n)$ at points $\Re(\lambda_1), ..., \Re(\lambda_n)$. Clearly $N = H + ip(H)$ and the claim follows. □

The property $\#\sigma(N) = \#\sigma(H)$ is not generic only in $\mathcal{N}$ but also in subsets of $\mathcal{N}$ that are relevant for our purposes.

Proposition 3 *The property $\#\sigma(N) = \#\sigma(H)$ is generic in*

$$\{N = H + iK \in \mathcal{N} | \#\sigma(N) = k\} \tag{12}$$

for every $1 \leq k \leq n$.

Proof. Let $\lambda_1, ..., \lambda_k$ denote the distinct eigenvalues of N, belonging to $\{N = H + iK \in \mathcal{N} | \#\sigma(N) = k\}$. Define a mapping

$$N \to \prod_{j=1}^{k-1} (\Im(\lambda_{j+1}) - \Im(\lambda_j)) \tag{13}$$

from $\{N = H + iK \in \mathcal{N} | \#\sigma(N) = k\}$ into $\mathbb{R}$. This is clearly continuous. The inverse image of 0 for (13) equals those $N \in \{N = H + iK \in \mathcal{N} | \#\sigma(N) = k\}$ for which $\#\sigma(N) > \#\sigma(H)$ which thereby is a closed set. To see that its complement is dense, rotations $e^{i\theta}N$ of N remain in (12). Choosing an arbitrarily small positive θ results in $\#\sigma(e^{i\theta}N) = \#\sigma(\frac{1}{2}(e^{i\theta}N + e^{-i\theta}N^*))$. □

Theorem 2 has a consequence as to solving iteratively linear systems involving normal matrices. To see this, we consider first the so-called ideal GMRES approximation problem [8]. For that purpose, assume having an invertible $A \in \mathbb{C}^{n \times n}$. By elementary linear algebra, $A^{-1} = p(A)$ for a polynomial p. Based on this, in the ideal GMRES approximation problem [8] one considers, for $1 \leq j \leq n - 1$,

$$\min_{p_{j-1} \in \mathcal{P}_{j-1}} \|Ap_{j-1}(A) - I\|, \tag{14}$$

where $\mathcal{P}_{j-1}$ denotes the set of polynomials of degree $j - 1$ at most. Typically the behavior of these quantities are of interest for small values of j compared

with the dimension n. The reason for this is that (14) is related to solving the linear system $Ax = b$, with a $b \in \mathbb{C}^n$, by using GMRES via

$$\min_{p_{j-1}\in\mathcal{P}_{j-1}} \|Ap_{j-1}(A)b - b\| \leq \min_{p_{j-1}\in\mathcal{P}_{j-1}} \|Ap_{j-1}(A) - I\|\|b\|. \tag{15}$$

For further details of GMRES algorithm and its relation to ideal GMRES problem, see e.g. [6, 18]. In addition to interest in behavior of (14) while j grows, there is a related property of A that governs the ultimate number of steps needed for solving $Ax = b$ exactly, at least in exact aritmethic. To this end, recall that the minimal polynomial of A is the monic polynomial of least degree annihilating A. Let $\deg(A)$ denote degree of the minimal polynomial of $A \in \mathbb{C}^{n\times n}$.

Proposition 4 *Let* $\deg(A)$ *denote the degree of the minimal polynomial of* $A \in \mathbb{C}^{n\times n}$. *Then* $A^{-1} = p(A)$ *for a polynomial of degree* $\deg(A) - 1$.

This is well-known and can be found e.g. from [16]. In particular, because of (15), after $\deg(A) - 1$ steps GMRES yields the solution.

Theorem 2 gives rise to a a problem analogous to ideal GMRES problem in the following manner. Namely, according to Theorem 2, a generic normal matrix N is a polynomial of its Hermitian part $H = \frac{1}{2}(N + N^*)$. Assuming N to be invertible, it holds that N^{-1} is a polynomial of N. Consequently, a generic normal invertible matrix N is a polynomial of its Hermitian part. By this deduction one easily derives an upper bound $(\deg(N)-1)^2$ for the degree of a polynomial yielding $N^{-1} = p(H)$. This, however, is far too pessimistic.

Theorem 5 *Assume* $N \in \mathcal{N}$ *is generic in the sense of Proposition 3. Then* $N^{-1} = p(H)$ *for a polynomial* p *of degree* $\deg(N) - 1$ *at most.*

Proof. Let $N = U\Lambda U^*$ be a diagonalization of N by a unitary matrix U so that its Toeplitz decomposition is as in (11). Since N is normal, there holds $\#\sigma(N) = \deg(N)$. Further, being generic in the sense of Proposition 3 means that $K = q(H)$ for a polynomial q and, consequently, $\deg(H) = \deg(N)$. Obviously the Toeplitz decomposition $N^{-1} = \hat{H} + i\hat{K}$ of N^{-1} is

$$N^{-1} = U \begin{bmatrix} \Re(1/\lambda_1) & & \\ & \ddots & \\ & & \Re(1/\lambda_n) \end{bmatrix} U^* + iU \begin{bmatrix} \Im(1/\lambda_1) & & \\ & \ddots & \\ & & \Im(1/\lambda_n) \end{bmatrix} U^*. \tag{16}$$

By interpolation, find a real polynomial p_1 that attains the values $\Re(1/\lambda_1), ..., \Re(1/\lambda_n)$ at points $\Re(\lambda_1), ..., \Re(\lambda_n)$. Then, analogously, find a real polynomial p_2 that attains the values $\Im(1/\lambda_1), ..., \Im(1/\lambda_n)$ at points $\Re(\lambda_1), ..., \Re(\lambda_n)$. The degree of both p_1 and p_2 is at most $\deg(N) - 1$. Furthermore, by construction $p(H) = p_1(H) + ip_2(H) = N^{-1}$ and the claim follows. □

Thus, since the inverse of $N \in \mathcal{N}$ is generically a polynomial of its Hermitian part, we are naturally led to consider, aside from the ideal GMRES problem,

$$\min_{p_{j-1} \in \mathcal{P}_{j-1}} \|Np_{j-1}(H) - I\|. \tag{17}$$

According to Theorem 5, this attains zero no later than the ideal GMRES does whenever N is generic. As with (14), for practical purposes the behavior of these quantities is of most interest for values of j far smaller than $\deg(N)-1$. Their behavior is easily understood as N is normal. Though, the problem of characterizing the convergence behavior of the ideal GMRES, as well as GMRES for solving $Ax = b$, using simple properties of A and b has received a lot attention, see [18, 6, 16] and references therein as well as more recent [15, 13, 11, 14]. From this point of view normal matrices are well-understood as the convergence can be characterized by solving polynomial approximation problems on the spectrum of N [7]. For (17) the corresponding approximation problems are just solved on the spectrum of H. Or, while approximating the inverse of N we have two *real* polynomial approximation problems as follows.

Corollary 6 *Let* p_1 *and* p_2 *solve* $\min_{p_{j-1} \in \mathcal{P}_{j-1}} \|\Re(\Lambda^{-1}) - p_{j-1}(\Lambda_H)\|$ *and* $\min_{p_{j-1} \in \mathcal{P}_{j-1}} \|\Im(\Lambda^{-1}) - p_{j-1}(\Lambda_H)\|$ *respectively. Then*

$$\min_{p_{j-1} \in \mathcal{P}_{j-1}} \|p_{j-1}(H) - N^{-1}\| = \|p_1(H) + ip_2(H) - N^{-1}\|.$$

Note that whenever N is Hermitian, then (17) reduces to the standard ideal GMRES problem for this Hermitian matrix. And the other way around, this is a continuous extension of the ideal GMRES for Hermitian matrices to the set of normal matrices. This extension is clearly not the same as (14) is.

Of course it is possible that a given $N \in \mathcal{N}$ is nongeneric in the sense that N is not a polynomial of its Hermitian part. This is the case, for instance, when N is skew-Hermitian as then the Hermitian part of N is the zero matrix. And more generally, when N has more than one eigenvalue on a vertical line. There is a simple trick that removes this problem. Namely, instead of N, consider $e^{i\theta}N$ for a $\theta \in [0, 2\pi)$. It is obvious that this rotation of N remains normal.

Theorem 7 *[12] Assume* $N \in \mathbb{C}^{n\times n}$ *is normal. Then, for* θ *belonging to an open dense subset of* $[0, 2\pi)$*, holds*

$$e^{i\theta}N = H_\theta + ip_\theta(H_\theta)$$

for $H_\theta = \frac{1}{2}(e^{i\theta}N + e^{-i\theta}N^*)$ *and a polynomial* p_θ *with real coefficients.*

By the same reasoning as earlier we have, for an invertible $N \in \mathcal{N}$ and for a θ belonging to an open dense subset of $[0, 2\pi)$,

$$N^{-1} = p_\theta(H_\theta) \tag{18}$$

for a polynomial p_θ. It is readily seen that the claim of Theorem 5 holds, i.e., the degree of p_θ in (18) is at most $\deg(N) - 1$, as well. However, it is not obvius how to pick a rotation θ yielding an optimal decay in the minimization problem (17). Still, since this rotation is important for our purposes, we set the following.

Definition 8 *Let $N \in \mathbb{C}^{n\times n}$ and $\theta \in [0, 2\pi)$. Then $N = e^{-i\theta}H_\theta + ie^{-i\theta}K_\theta$ is the rotated Toeplitz decomposition of N by the angle θ.*

In this decomposition the parts are typically not Hermitian matrices. This is obviously irrelevant as all the computational aspects are analogous for H_θ and $e^{-i\theta}H_\theta$. Recall that matrices H_θ arise while approximating the field of values of a (not necessarily normal) matrix N. Namely then, for a finite number of different θ, one computes the largest eigenvalue of H_θ and intersects certain half-planes defined on the basis of these eigenvalues, see e.g. [10][Thm 1.5.12, 1.5.14].

3 A Hermitian Lanczos for solving $Nx = b$

Consider solving iteratively, with a given $b \in \mathbb{C}^n$, a linear system

$$Nx = b, \tag{19}$$

for a large, possibly sparse, invertible matrix $N \in \mathcal{N}$. If N is Hermitian, then this can be accomplished by an optimal method based on a 3-term recurrence, see e.g. [6]. If N is non-Hermitian normal matrix, then the recurrencies for an optimal approximation are generically long by the result of Faber and Manteuffel [4]. Their result states that there is an optimal recurrence of length $\deg(p) + 2$, where p is the degree of the polynomial yielding $N^* = p(N)$. That for a normal N there holds $N^* = p(N)$ for a polynomial p is the condition 17 in [9]. Irritatively though, the length of a recurrence is a very noncontinuous property among the set normal matrices.

EXAMPLE 1. Consider a Hermitian invertible $H \in \mathbb{C}^{n\times n}$ and solving iteratively a system $Hx = b$ for $b \in \mathbb{C}^n$. This can be done by using a 3-term recurrence. However, let us slightly perturb H in a very simple manner, for instance, set $N = H + i\alpha H^2$, where $\alpha > 0$ is a small parameter. Then N is not quite Hermitian anymore and the spectrum of N does not lie on a line but it is slightly concave down. This small perturbation has destroyed the optimality of the used 3-term recurrence.

An optimal 3-term recurrence for solving a linear system, whenever N^* is available, is always obtained by executing the CGN method, the CG for the normal equations. That is, by solving, instead of (19), the system

$$N^*Nx = N^*b \text{ or } NN^*y = b \text{ with } x = N^*y \tag{20}$$

using CG method. It is well-known that this approach may not be a good idea although it is not clear when it is so. The squared conditioning of the resulting systems (20) is the most standard argument against the CGN.

In what follows we derive a 3-term recurrence for solving (19) that does not use normal equations and does not lead to squared condition number. To this end, in order to obtain an iterative method, we replace (17) with a minimization problem involving the vector b. That is, we consider, as in GMRES,

$$\min_{p_{j-1}\in\mathcal{P}_{j-1}} \|Np_{j-1}(H)b - b\| \tag{21}$$

with $H = \frac{1}{2}(N + N^*)$. As the relation (15) between GMRES and the ideal GMRES, there is an anlogous relation between (17) and (21). Consequently, using the notation of Corollary 6, the decay of (21) can be bound by the complex approximation problem

$$\min_{p_{j-1}\in\mathcal{P}_{j-1}} \|Np_{j-1}(H)b - b\| \leq \min_{p_{j-1}\in\mathcal{P}_{j-1}} \|\Lambda p_{j-1}(\Lambda_H) - I\|\|b\| \tag{22}$$

on the spectrum of H. Since

$$\min_{p_{j-1}\in\mathcal{P}_{j-1}} \|\Lambda p_{j-1}(\Lambda_H) - I\| \leq \|N\| \min_{p_{j-1}\in\mathcal{P}_{j-1}} \|p_{j-1}(\Lambda_H) - \Lambda^{-1}\| \tag{23}$$

the convergence can also be bounded by considering two real approximation problems on the spectrum of H, see Corollary 6.

Since N commutes with H, (21) is equal to

$$\min_{p_{j-1}\in\mathcal{P}_{j-1}} \|p_{j-1}(H)Nb - b\| \tag{24}$$

the value of which is readily obtained with a Krylov subspace method. That is, finding (24) is equivalent with approximating b from the Krylov subspace

$$\mathcal{K}_j(H; Nb) = \text{span}\{Nb, HNb, ..., H^{j-1}Nb\}. \tag{25}$$

An inexpensive way to realize this is to execute the Hermitian Lanczos method with H starting from $\hat{q}_0 = \frac{Nb}{\|Nb\|}$. The Hermitian Lanczos method is a well-known algorithm that transforms a Hermitian matrix to a tridiagonal matrix. It is realized by computing, with a Hermitian H, using an initial vector $q_0 \in \mathbb{C}^n$

$$T_j := Q_j^* H Q_j = \begin{bmatrix} \alpha_1 & \beta_1 & 0 & & \\ \beta_1 & \alpha_2 & \beta_2 & & \\ 0 & \beta_2 & \ddots & \ddots & \\ & & \ddots & \alpha_{j-1} & \beta_{j-1} \\ & & & \beta_{j-1} & \alpha_j \end{bmatrix} \tag{26}$$

where $Q_j \in \mathbb{C}^{n\times j}$ has orthonormal columns spanning the Krylov subspace

$$\mathcal{K}_j(H; q_0) = \text{span}\{q_0, Hq_0, H^2q_0, ..., H^{j-1}q_0\}. \tag{27}$$

The elements of the matrix (26) are computed by using the 3-term recursion

$$\beta_j q_j = Hq_{j-1} - (Hq_{j-1}, q_{j-1})q_{j-1} - (Hq_{j-1}, q_{j-2})q_{j-2}, \tag{28}$$

where β_j equals the norm of the right-hand side of (28). For further details of the Hermitian Lanczos, see e.g. [1, 19, 17, 5].

To solve (24), we formally start the iteration from $\hat{q}_0 = \frac{Nb}{\|Nb\|} \in \mathbb{C}^n$ as

$$\|p(H)Nb - b\| = \|Nb\|\|p(H)\frac{Nb}{\|Nb\|} - \frac{b}{\|Nb\|}\| \tag{29}$$

for every polynomial p. The standard Hermitian Lanczos iteration (28) would then proceed as

$$\hat{q}_1 = \frac{1}{\beta_1}\big(H\hat{q}_0 - (H\hat{q}_0, \hat{q}_0)\hat{q}_0\big) \tag{30}$$

$$\hat{q}_2 = \frac{1}{\beta_2}\big(H\hat{q}_1 - (H\hat{q}_1, \hat{q}_1)\hat{q}_1 - (H\hat{q}_1, \hat{q}_0)\hat{q}_0\big) \tag{31}$$

$$\vdots$$

so that at the j^{th} step one computes

$$\hat{q}_j = \frac{1}{\beta_j}\big(H\hat{q}_{j-1} - (H\hat{q}_{j-1}, \hat{q}_{j-1})\hat{q}_{j-1} - (H\hat{q}_{j-1}, \hat{q}_{j-2})\hat{q}_{j-2}\big). \tag{32}$$

The constants β_k's are chosen such that $\|\hat{q}_j\| = 1$ for $0 \leq k \leq j$. Then, obviously,

$$\min_{p_j \in \mathcal{P}_j} \|p_j(H)Nb - b\| = \|Nb\| \min_{p_j \in \mathcal{P}_j} \|p_j(H)\frac{Nb}{\|Nb\|} - \frac{b}{\|Nb\|}\| \tag{33}$$

is realized by the polynomial p_j fulfilling

$$p_j(H)\frac{Nb}{\|Nb\|} = \sum_{k=0}^{j} (\frac{b}{\|Nb\|}, \hat{q}_j)\hat{q}_j \tag{34}$$

as the vectors $\{\hat{q}_k\}_{k=0}^{j}$ are orthonormal. The problem is that this scheme does not yield a solution candidate x_j for solving the linear system $Nx = b$. Instead, it yields the minimum value (24), so that the vector (34) should be multiplied by $\|Nb\|N^{-1}$ to get the approximation x_j. To avoid inversion, the trick is that, since

$$x_j = \|Nb\| \sum_{k=0}^{j} (\frac{b}{\|Nb\|}, \hat{q}_k)N^{-1}\hat{q}_k = \sum_{k=0}^{j} (b, \hat{q}_k)N^{-1}\hat{q}_k, \tag{35}$$

we do not actually compute (30), (31) and (32). Instead, we set $q_0 = \frac{b}{\|Nb\|}$ and

$$q_1 := N^{-1}\hat{q}_1 = \frac{1}{\beta_1}\big(Hq_0 - (H\hat{q}_0, \hat{q}_0)q_0\big) \tag{36}$$

$$q_2 := N^{-1}\hat{q}_2 = \frac{1}{\beta_2}\big(Hq_1 - (H\hat{q}_1, \hat{q}_1)q_1 - (H\hat{q}_1, \hat{q}_0)q_0\big) \tag{37}$$

$$\vdots$$

so that at the j^{th} step we have

$$q_j := N^{-1}\hat{q}_j = \frac{1}{\beta_j}\big(Hq_{j-1} - (H\hat{q}_{j-1}, \hat{q}_{j-1})q_{j-1} - (H\hat{q}_{j-1}, \hat{q}_{j-2})q_{j-2}\big). \tag{38}$$

At each step the inner-products only formally involve $\hat{q}_k$'s as they can be computed by using the relation $Nq_k = \hat{q}_k$. Consequently, only vectors of the form q_k are saved and the arisen recurrence relies only on 3 vectors as (35) yields an update

$$x_j = \sum_{k=0}^{j}(b, Nq_j)q_j = x_{j-1} + (b, Nq_j)q_j. \tag{39}$$

Thus we have obtained the following basic algorithm.

Algorithm 1. "For solving $Nx = b$".
For $N = H + iK \in \mathcal{N}$ and a vector b set $H = \frac{1}{2}(N + N^*)$, $q_0 = \frac{b}{\|Nb\|}$, $q_{-1} = 0$ and $x_0 = (b, Nq_0)q_0$.
For $j = 1$ to k compute
$q_j = Hq_{j-1} - (HNq_{j-1}, Nq_{j-1})q_{j-1} - (HNq_{j-1}, Nq_{j-2})q_{j-2}$
$q_j = \frac{q_j}{\|Nq_j\|}$
$x_j = x_{j-1} + (b, Nq_j)q_j$
end for.

Remark 1. As opposed to the CGN method, the proposed scheme does not square the condition number as H is formed via a (weighted) summation, not multiplication. Another consequence of the summation is that the scheme reduces to GMRES whenever N is Hermitian.

Remark 2. In addition to the complexity of the standard Hermitian Lanczos iteration step (32), additional 3 matrix-vector products Nq_{j-2}, Nq_{j-1} and Nq_j are needed while computing q_j.

Remark 3. The computed vectors $\{q_k\}_{k=0}^{j}$ themselves need not be orthonormal but $\{Nq_k\}_{k=0}^{j}$ are.

Remark 4. It is straighforward to modify the above algorithm such that an initial guess x_{-1} is used instead. That is, then b is replaced with the residual $r = b - Nx_{-1}$ and $q_0 = \frac{r}{\|Nr\|}$ taken to be the starting vector. Then the approximative solution is, at the k^{th} step, $\hat{x}_k = x_{-1} + x_k$.

Remark 5. Because of (18), it is possible to use a rotated Toeplitz decomposition of N instead. This means simply replacing H with H_θ in the above algorithm.

Remark 6. Combining Remarks 4 and 5 gives a scheme in which the rotation parameter θ is varied during the iteration. That is, the iteration is started with a θ_0 and with an initial guess x_{-1}. Then the algorithm is executed, with $r = b - Nx_{-1}$ in place of b, $q_0 = \frac{r}{\|Nr\|}$ and with H_θ in place of H. After, let us say, k steps the algorithm has produced x_k so that an approximative solution $\hat{x}_k = x_{-1} + x_k$ is obtained. Then another rotation parameter θ_1 is chosen, in case of stagnation for instance, and the scheme is restarted by using the just computed $\hat{x}_k$ as an initial guess. We will consider this more below.

Let us formulate, aside form the basic Algorithm 1, an algorithm resulting from Remark 6.

Algorithm 2. "For solving $Nx = b$".
For $N = e^{-i\theta}H_\theta + ie^{-i\theta}K_\theta \in \mathcal{N}$ *and an initial guess* x_{-1} *set* $r = b - Nx_{-1}$, $q_0 = \frac{r}{\|Nr\|}$, $q_{-1} = 0$ *and* $x_0 = (b, Nq_0)q_0$.
For $j = 1$ *to* k *compute*
$q_j = H_\theta q_{j-1} - (H_\theta Nq_{j-1}, Nq_{j-1})q_{j-1} - (H_\theta Nq_{j-1}, Nq_{j-2})q_{j-2}$
$q_j = \frac{q_j}{\|Nq_j\|}$
$x_j = x_{j-1} + (b, Nq_j)q_j$
end for.
$\hat{x}_k = x_{-1} + x_k$.
Rstart with a new θ.

Remark 7. The usage of restarts and rotations suggested in Remark 6 removes the nongenericity problem of $N \in \mathcal{N}$ not being a polynomial of its Hermitian part. A simple way to achieve this is to monitor the size of updates $(b, Nq_j)q_j$. If the updates remain under a threshold for a number a consecutive steps and the approximative solution is not sufficiently accurate, then another θ is introduced and the so far computed approximation is used as an initial guess. Thereby no gained information is lost.

Remark 8. In a nearly nongeneric case the convergence can slow down for a while unless rotations and restarts are used. This is readily explained by the bound (23) and Corollary 6. Namely then the Hermitian part of N has has close eigenvalues and therefore the approximation polynomials p_1 and p_2 of Corollary 6 may need to make violent turns over a short interval in order to approximate $\Re(\Lambda^{-1})$ and $\Im(\Lambda^{-1})$ well. We strongly recommend using restarts and rotations in these cases. The convergence can be very good with extremely thick restarts combined with random rotations, see numerical examples of Section 4.

Remark 9. As with the original the Hermitian Lanczos method, also Algorithm 1 suffers from loss of orthogonality (of vectors $\{Nq_k\}_{k=0}^{j}$ in Remark 3) resulting from finite precision and short term recurrencies. This is a problem in eigenvalue approximations in particular. Standard tricks against this are full-orthogonalization or selective orthogonalization [17, 1]. But then,

obviously, the memory requirements increase accordingly.

Remark 10. As the underlying minimization problem is (17), also other information could be extracted from the iteration process, like location of eigenvalues. An algorithm was derived in [12] and from (21) it is possible to derive another type of algorithm. We do not consider this problem here.

Let us illustrate Remark 7 more thoroughly with a simple *nongeneric* example.

EXAMPLE 2. Let $N = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & i & 0 \\ 0 & 0 & 0 & -i \end{bmatrix}$ and $b = \begin{bmatrix} \frac{1}{2} \\ \frac{1}{2} \\ \frac{1}{2} \\ \frac{1}{2} \end{bmatrix}$. Thus N is nongeneric as $\#\sigma(H) = 3 < 4 = \#\sigma(N)$. A simple computation gives

$$\mathcal{K}_3(H; Nb) = \mathcal{K}_4(H; Nb) = \text{span}\{ \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ 0 \\ \frac{1}{\sqrt{2}} \\ \frac{-1}{\sqrt{2}} \end{bmatrix} \}.$$

Therefore Algorithm 1 yields $x_3 = \begin{bmatrix} \frac{1}{2} \\ -\frac{1}{2} \\ 0 \\ 0 \end{bmatrix}$ and $Nx_3 = \begin{bmatrix} \frac{1}{2} \\ \frac{1}{2} \\ 0 \\ 0 \end{bmatrix}$ so that $r = b - Nx_3 = \begin{bmatrix} 0 \\ 0 \\ \frac{1}{2} \\ \frac{1}{2} \end{bmatrix}$. Next we set $q_0 = \frac{r}{\|Nr\|}$ and x_3 to be the intial guess. We choose $\theta_1 = \frac{\pi}{2}$ so that according to Remark 6, with q_0, x_3 and $H_{\frac{\pi}{2}}$, we obtain

$$\mathcal{K}_2(H_{\frac{\pi}{2}}; Nr) = \mathcal{K}_3(H_{\frac{\pi}{2}}; Nr) = \text{span}\{ \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix} \}.$$

Thus $y_2 = \begin{bmatrix} 0 \\ 0 \\ -\frac{i}{2} \\ \frac{i}{2} \end{bmatrix}$ and $Ny_2 = \begin{bmatrix} 0 \\ 0 \\ \frac{1}{2} \\ \frac{1}{2} \end{bmatrix}$. In particular, we obtain the solution as $N(x_3 + y_2) = b$.

Although also the rotation resulted in nongeneric $e^{i\frac{\pi}{2}}N$, the solution was obtained after one restart. An interesting problem is how to rotate N during the iteration to achieve the fastest possible convergence. It is interesting to note that as such, while using rotations, the method is not quite a Krylov subspace method. As to Algortihm 1, its convergence for Hermitian H is the same as GMRES and for most rotations of H this is true as well.

Proposition 9 *Assume $H \in \mathcal{H}$ and $b \in \mathbb{C}^n$. Then the convergence of Algorithm 1 for solving $e^{i\theta}Hx = b$ is independent of $\theta \in [0, 2\pi)\backslash\{\frac{\pi}{2}, \frac{3\pi}{2}\}$.*

Proof. This follows from the property that

$$\mathcal{K}_j(H_\theta; e^{i\theta}Hb) = \text{span}\{Hb, HHb, ..., H^{j-1}Hb\}.$$

as long as $\theta \in [0, 2\pi)\backslash\{\frac{\pi}{2}, \frac{3\pi}{2}\}$. Easiest way to verify this is to diagonalize H first by a unitary similarity. Thus, by (24), the claim follows. □

To end with, one can argue that solving linear systems involving normal matrices is too specific a problem. However, the first argument against this point is that before even considering mastering nonnormal problems, we have tried to gain understanding of solving systems with normal matrices. Second, there also arises the possibility of using normal matrices while preconditioning nonnormal problems as they can be solved with modest memory requirements with the proposed algorithm. Third, minimal decomposition, i.e., finding for a given $A \in \mathbb{C}^{n\times n}$ a splitting $A = N + F$ with a normal N such that F is of least possible rank, is also of interest besides from the point of view of analysis [15]. Namely, whenever the splitting $A = N + F$ of A is regular, any linear system $Ax = b$, with $b \in \mathbb{C}^n$, can be solved using inner-outer iterations such that the number of outer iterations depends on the rank of F directly. For more details, see [15, 14].

4 Numerical experiments

Next we consider numerical experiments for solving $Nx = b$. Our matrices are relatively small as we have prefered well-known examples to illustrate how Algorithms 1 and 2 extends GMRES *and* how to use restarts suggested in Remarks 6 and 7. The computations are performed with Matlab and we use its syntax while explainig the numerical examples. In all the examples $N \in \mathbb{C}^{n\times n}$ is normal and, unless otherwise stated, $b \in \mathbb{C}^n$ is a random complex vector, that is $b = \text{rand}(n, 1) + i\text{rand}(n, 1)$.

EXAMPLE 3. We start with a very well understood example illustrating how Algorithm 1 extends GMRES for Hermitian matrices to normal matrices in a continuous way. We compare the convergence for $N_0 = H = \text{diag}(8(6+\text{randn}(600, 1))) \in \mathbb{C}^{600\times 600}$ with Hermitian positive definite H and for a "slightly" bent N_0, that is, for $N_j = H + i\alpha_j H^2$, with small positive α_j's. Besides $\alpha_0 = 0$, we set $\alpha_1 = 0.01$, $\alpha_2 = 0.1$ and $\alpha_3 = 1$. Note that for N_0 Algorithm 1 is GMRES. In Figure 4.1 we have depicted the eigenvalues of N_0, N_1 and N_2 and N_3. Note that N_0, N_1, N_2 and N_3 are not close. Still, from Figure 4.2, where we have plotted relative residuals $\|b - Nx_k\|/\|b\|$, we observe that the convergence of Algorithm 1 is very similar for these matrices.

EXAMPLE 4. This example illustrates the effect of rotations combined with initial guesses as suggested in Remark 6. We define N via $N = \text{diag}([n1; n2; n3; n4])$, where $n1 = 3(5+\text{randn}(100, 1))$, $n2 = 5(-7+\text{randn}(100, 1))$, $n3 = 4(6 + \text{randn}(100, 1))i$ and $n4 = 2(-10 + \text{randn}(100, 1))i$. Thus, $N \in \mathbb{C}^{400\times 400}$ and its spectrum lies on the union of x- and y-axis like a "cross", see

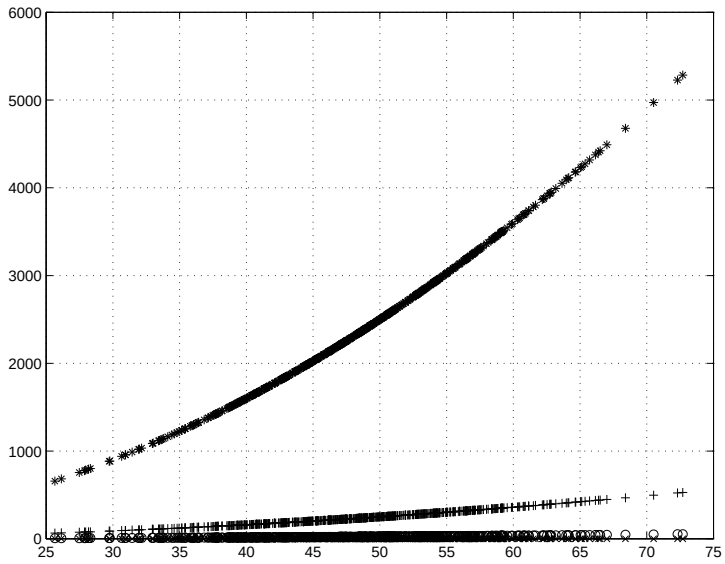

Figure 1: The eigenvalues of the matrices N_0, N_1, N_2 and N_3 of Example 3 are denoted by 'x', 'o', '$+$' and '$*$' respectively.

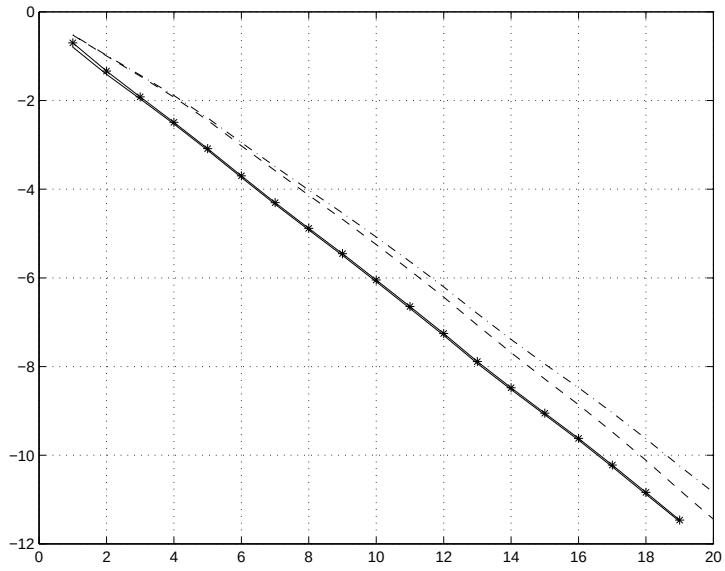

Figure 2: The convergence of relative residuals for Algorithm 1 in log10-scale for Example 3. The convergence is denoted by '$-$', '$-*$', '$--$' and '$-\cdot$' for N_0, N_1 and N_2 and $N3$ respectively.

Firgure 4.3. In particular, N is nongeneric as there are several eigenvalues on a vertical line, that is, on the y-axis. This is a difficult problem for GMRES as a lot of iterations are needed. We perform 80 steps which a very large amount taking into account the dimension. We use the following rotation choices with Algorithm 2:
20-20 is such that we take 20 steps with H and then rotate by $\frac{\pi}{2}$ and take

20 steps with $H_{\frac{\pi}{2}}$. This is then repeated.
Random-5 is such that we take a random rotation and perform 5 step and take another random rotation and perform 5 steps. This is then repeated.
8-8 is such that we take 8 steps with H and then rotate by $\frac{\pi}{2}$ and take 8 steps with $H_{\frac{\pi}{2}}$. This is then repeated.

In Figure 4.4 we have plotted relative residuals $\|b - Nx_k\|/\|b\|$ of GMRES and each 3 strategies above.

Let us try to explain the dependence of the convergence on rotations for **20-20** and **8-8**. Starting with $\theta_0 = 0$ means that H_0 does not posess any information of the eigenvalues on the imaginary axis. Thus, then the iteration behaves nearly like GMRES for the Hermitian $\mathrm{diag}([n1; n2])$ and decreases error in the corresponding subspace of dimension 200. After stagnation, the corresponding projected problem onto that subspace is approximatively solved. If a rotation $\theta_1 = \frac{\pi}{2}$ is then made, using the obtained solution candidate as an initial guess, then the iteration behaves nearly like GMRES for the Hermitian $\mathrm{diag}([n3/i; n4/i])$ and decreases error in the corresponding subspace of dimension 200.

Note that **Random-5** decreases the residual like (full) GMRES.

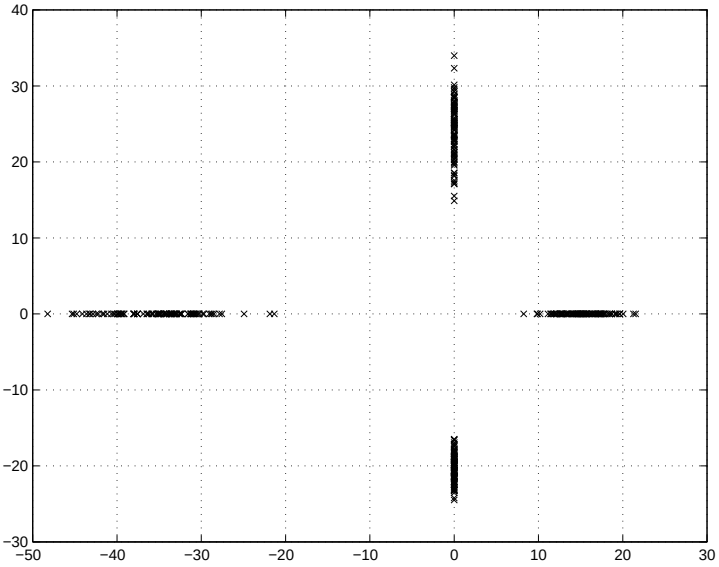

Figure 3: The eigenvalues of the matrix N in Example 4.

EXAMPLE 5. We let $N \in \mathbb{C}^{500\times 500}$ to be the notorious unitary shift and b a standard unit basis vector. Thus, the origin is surrounded by the eigenvalues of N, see Figure 4.5. Although being an easy problem for CGN [6], this is a very diffucult problem for GMRES. It is well-know that the convergence of GMRES for this starting vector is catastrophic as it makes no progress before n^{th} step. As there are no angles to prefer, we use very thick restarts with random rotations. That is, we use **Random-1** and **Random-3** strategies explained in Example 4. The convergence of relative residuals $\|b - Nx_k\|/\|b\|$

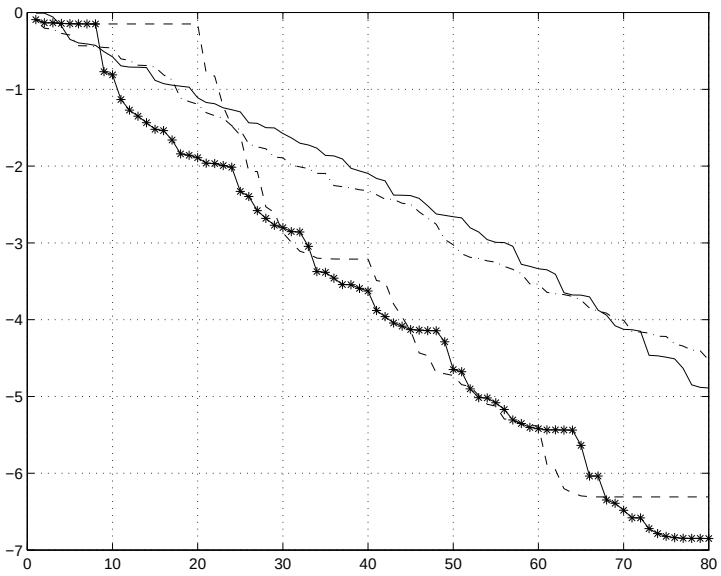

Figure 4: The convergence of relative residuals for in log10-scale for Example 4. Solid line is GMRES and '$--$' is **20-20**, '$-\cdot$' is **random-5** and '$-*$' is **8-8**.

is depicted in Figure 4.6. Surpricingly, very thick restarting seems to be a good choice for this example.

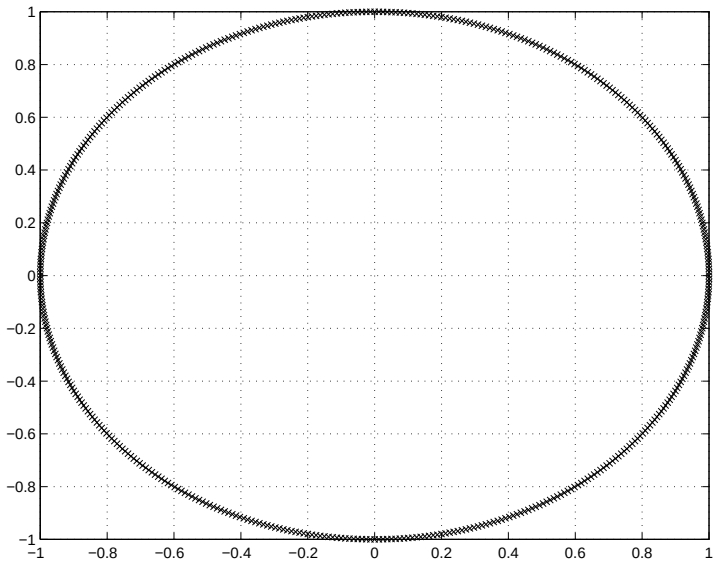

Figure 5: The eigenvalues of the matrix N in Example 5.

EXAMPLE 6. We set $N = I + 0.1\text{diag}(\text{randn}(100,1) + i\text{randn}(100,1)) \in \mathbb{C}^{100\times 100}$. As opposed to Example 5, this matrix is particularly favourable to GMRES since N has a very concentrated spectrum around 1. The spectrum

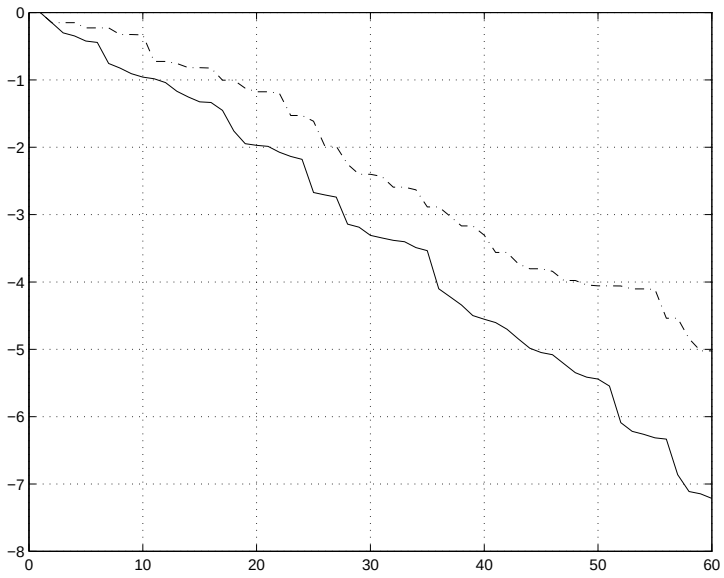

Figure 6: The convergence of relative residuals for in log10-scale for Example 5. Solid line is **Random-1** and '−·' is **Random-3**.

is otherwise very unstructured so that there is no direction to prefer with Algorithm 1 and polynomial interpolation for the Hermitian part can be troublesome. We use therefore Algorithm 2 with thick restarts by using again **Random-1** and **Random-3** strategies explained in Example 4. Observe from Figure 4.7 that **Random-1** wins.

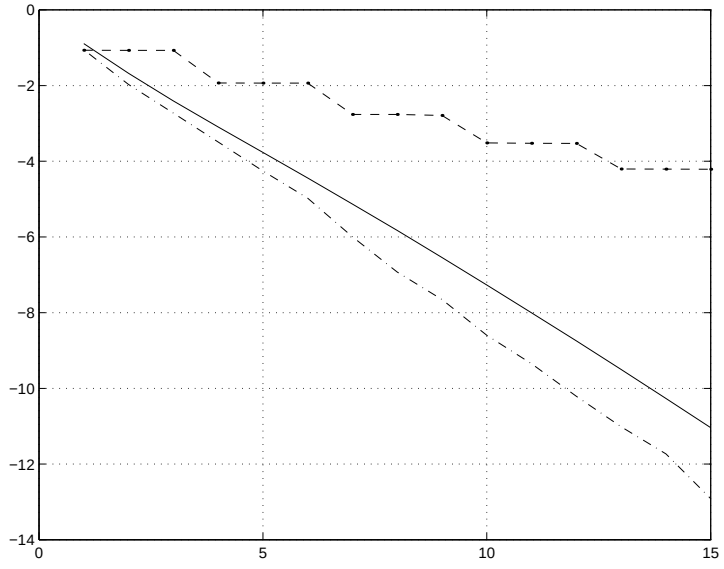

Figure 7: The convergence of relative residuals for in log10-scale for Example 6. Solid line is GMRES, '−·' is **Random-1** and '−−' is **Random-3**.

5 Conclusions

In this paper we have derived a Hermitian Lanczos method for solving a linear system $Nx = b$ involving a normal matrix N. The obtained method is optimal when measured in a way that resembles the definition of GMRES. The algorithm is realizable with a 3-term recurrence and reduces to GMRES whenever N is Hermitian. Furthermore, rotations and restarts play an extremely important role in the convergence behavior of the introduced method. We have illustrated this with numerical examples. If there is information about the spectrum, then rotations should be chosen such that parts of the spectrum are well approximated by polynomials if possible. Unless there is information about the spectrum of N, we do not know how to optimally choose rotations as well as thickness of restarts. However, thick restarting combined with random rotations seems to a very good alternative then.

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