The Lanczos reduction to semiseparable matrices

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Abstract - An algorithm that transforms symmetric matrices into similar semiseparable ones has been proposed recently. Similarly to the Householder reduction, the latter algorithm works without taking into account the structure of the original matrix. In this paper we propose a Lanczos–like algorithm to transform a symmetric matrix into a similar semiseparable one relying on the product of the original matrix times a vector at each step. Therefore an efficient algorithm can be considered if the original matrix is sparse or structured.

Keywords— **Lanczos algorithm, semiseparable matrix, rehortogonalization, rank revealing.**

I. INTRODUCTION

An algorithm that transforms symmetric matrices into similar semiseparable ones has been proposed recently [VAN 05]. The algorithm combines the properties of the Lanczos tridiagonalization [GOL 96, pp. 470–499] with those of the subspace iteration method [GOL 96, pp. 332–334], with the size of the subspace increasing by one dimension at each step of the algorithm. Hence, in many cases, after a few steps of the algorithm, the eigenvalues, and the corresponding eigenvectors, are already well approximated. Unfortunately, similarly to the Householder reduction, the latter algorithm destroys the structure of the original matrix.

In this paper we propose a Lanczos–like algorithm to transform a symmetric matrix into a similar semiseparable one that, similarly to the Lanczos tridiagonalization, relies on the product of the original matrix times a vector at each step. Therefore it can be efficiently used if the original matrix is sparse or structured.

The matrices handled in this paper are symmetric. However, there is no loss of generality, because it will be shown that similar techniques can be applied to real unsymmetric matrices, as well. Moreover, the extension of this algorithm to reduce rectangular matrices into upper triangular semiseparable ones in order to compute the singular value decomposition [VAN 04b] is quite straightforward.

As an application, the proposed algorithm has been considered for computing the kernel step of a state–space method called HLSVD [TUF 82], [LAU 02], [LAU 05], in which the subspace associated to the largest singular values of a Hankel matrix is computed.

The paper is organized as follows. In section II the basic steps of the classical Lanczos algorithm are described followed by the Lanczos algorithm for reducing symmetric matrices into semiseparable ones. Some numerical experiments are shown in section III followed by the conclusions and future work.

II. LANCZOS–LIKE ALGORITHM FOR SEMISEPARABLE MATRICES

The Lanczos algorithm is a simple and effective method for finding extreme eigenvalues and corresponding eigenvectors of symmetric matrices. Because it only accesses the matrix through matrix–vector multiplications, it is commonly used when matrices are sparse or structured. The algorithm can be summarized in the following steps.

Lanczos algorithm
$A \in \mathbb{R}^{n\times n}$ symmetric and $r_0 \in \mathbb{R}^n$ the initial guess.
$\beta_0 = \|r_0\|_2$ and $q_0 = 0$.
`for` $i = 1, 2, \ldots$
(a) $q_i = r_{i-1}/\|r_{i-1}\|_2$
(b) $p = Aq_i$
(c) $\alpha_i = q_i^T p$
(d) $r_i = p - \alpha_i q_i - \beta_{i-1} q_{i-1}$
(e) $\beta_i = \|r_i\|_i$

Let $Q_k \equiv [q_1, q_2, \ldots, q_k]$ and

$$T_k = \begin{bmatrix} \alpha_1 & \beta_1 & & & \\ \beta_1 & \alpha_2 & \beta_2 & & \\ & \beta_2 & \ddots & \ddots & \\ & & \ddots & \alpha_{n-1} & \beta_{k-1} \\ & & & \beta_{k-1} & \alpha_k \end{bmatrix},$$

and let $T_k = U_k \Theta_k U_k^T$ its spectral decomposition, with $\Theta_k = \mathrm{diag}(\theta_1, \theta_2, \ldots, \theta_k)$ and $U_k \in \mathbb{R}^{k\times k}$ orthogonal. Then

$$A(Q_k U_k) = (Q_k U_k)\Theta_k + \beta_k q_{k+1} e_k^T U_k,$$

where e_k is the last vector of the canonical basis of $\mathbb{R}^k$. It turns out (see, e.g., [GOL 96, pp. 475]) that

$$\min_{\mu\in\lambda(A)} |\theta_i - \mu| \leq |\beta_k||u_{k,i}|, \quad i = 1, \ldots, k.$$

Hence β_k and the last components of the eigenvectors of T_k associated to θ_i give an indication on the convergence of the latter eigenvalues to the eigenvalues of A.

To prevent the loss of orthogonality in the computation of the Krylov basis Q_k, a lot of techniques have been developed (see, e.g., [GOL 96] and the references therein, [PAI 71], [PAR 79], [SIM 84a], [SIM 84b]).

The Lanczos-like algorithm for semiseparable matrices is based on the classical Lanczos algorithm for reducing symmetric matrices into similar symmetric tridiagonal ones [VAN 05].

Before considering it, let us introduce the definition of generator representable semiseparable matrices.

Definition 1: A matrix S is called a generator representable semiseparable matrix if

$$S = \begin{bmatrix} v_1u_1 & v_1u_2 & v_1u_3 & \ldots & v_1u_n \\ v_1u_2 & v_2u_2 & v_2u_3 & \ldots & v_2u_n \\ v_1u_3 & v_2u_3 & \ddots & \ddots & \vdots \\ \vdots & \vdots & \ddots & \ddots & \vdots \\ v_1u_n & v_2u_n & \cdots & \cdots & v_nu_n \end{bmatrix},$$

i.e., the lower triangular part is equal to the lower triangular part of the rank–one matrix uv^T and, symmetrically, the upper triangular part is equal to the upper triangular part of vu^T. The vectors $u = [u_1, \ldots, u_n]^T$ and $v = [v_1, \ldots, v_n]^T$ are the generators of S.

Remark 1: A semiseparable matrix is a block diagonal matrix, whose diagonal blocks are generator representable semiseparable matrices.

Remark 2: A comprehensive treatment of *semiseparable–like* matrices can be found in [VAN 04a]. A more stable end efficient representation of semiseparable matrices in the context of eigenvalue problems can be found in the latter reference as well.

Given $A \in \mathbb{R}^{n\times n}$, the ith step, $i = 1, ..., n-1$, of the algorithm described in [VAN 05] to reduce a symmetric matrix into a symmetric semiseparable one can be summarized as follows.

Reduction of a symmetric matrix into symmetric semiseparable form

Let $A_0 \equiv A$.

`for` $i = 1, \ldots, n-1$,

(a) Compute the Householder matrix H_i in order to annihilate the entries of A_{i-1} in the ith column below the $(i+1)$th row.

(b) Compute $H_iA_{i-1}H_i^T$

(c) Compute the orthogonal matrix Z_i such that the leading principal submatrix of order $i+1$ of $Z_iH_iA_{i-1}H_i^TZ_i^T$ is symmetric semiseparable

(d) $A_i = Z_iH_iA_{i-1}H_i^TZ_i^T$

Remark 3: The leading principal submatrices of order i of $H_iA_{i-1}H_i^T$ have already the symmetric semiseparable structure. Therefore step (c) in the latter algorithm can be interpreted as an updating step, i.e., increasing by one the order of the leading principal semiseparable submatrix.

A. Updating of semiseparable matrices

Let $S_k \in \mathbb{R}^{k\times k}$ be a symmetric semiseparable matrix. We describe now how the augmented matrix

$$\hat{S}_{k+1} = \left[\begin{array}{ccccc|c} & & & & & 0 \\ & & S_k & & & \vdots \\ & & & & & 0 \\ & & & & & \beta_k \\ \hline 0 & \cdots & 0 & \beta_k & & \alpha_{k+1} \end{array}\right], \qquad (1)$$

with $\beta_k \neq 0$, can be updated, i.e., reduced in symmetric semiseparable form by orthogonal similarity transformations working on the first k rows (and columns).

For simplicity, let us suppose $k = 4$,

$$\hat{S}_5 = \left[\begin{array}{cccc|c} u_1v_1 & u_1v_2 & u_1v_3 & u_1v_4 & 0 \\ u_1v_2 & u_2v_2 & u_2v_3 & u_2v_4 & 0 \\ u_1v_3 & u_2v_3 & u_3v_3 & u_3v_4 & 0 \\ u_1v_4 & u_2v_4 & u_3v_4 & u_4v_4 & \beta_4 \\ \hline 0 & 0 & 0 & \beta_4 & \alpha_5 \end{array}\right].$$

Define $\delta_4 \equiv \beta_4$. Let $\hat{G}_3$ be the Givens rotation

$$G_3 = \begin{bmatrix} c_3 & s_3 \\ -s_3 & c_3 \end{bmatrix}$$

such that

$$G_3 \begin{bmatrix} v_3 \\ v_4 \end{bmatrix} = \begin{bmatrix} \hat{v}_3 \\ 0 \end{bmatrix}$$

and let

$$\hat{G}_3 = \begin{bmatrix} I_2 & & \\ & G_3 & \\ & & I_1 \end{bmatrix},$$

where I_k is the identity matrix of order k. Then,

$$\hat{G}_3\hat{S}_5 = \begin{bmatrix} u_1v_1 & u_1v_2 & u_1v_3 & u_1v_4 & 0 \\ u_1v_2 & u_2v_2 & u_2v_3 & u_2v_4 & 0 \\ u_1\hat{v}_3 & u_2\hat{v}_3 & u_3\hat{v}_3 & \rho_3 & s_3\delta_4 \\ 0 & 0 & 0 & \delta_3 & c_3\delta_4 \\ 0 & 0 & 0 & \delta_4 & \alpha_5 \end{bmatrix},$$

with

$$\begin{bmatrix} \rho_3 \\ \delta_3 \end{bmatrix} = \begin{bmatrix} (c_3u_3 + s_3u_4)v_4 \\ (-s_3u_3 + c_3u_4)v_4 \end{bmatrix}.$$

Therefore

$$\begin{aligned} S_5^{(1)} &\equiv \hat{G}_3\hat{S}_5\hat{G}_3^T \\ &= \begin{bmatrix} u_1v_1 & u_1v_2 & u_1\hat{v}_3 & 0 & 0 \\ u_1v_2 & u_2v_2 & u_2\hat{v}_3 & 0 & 0 \\ u_1\hat{v}_3 & u_2\hat{v}_3 & \eta_3 & s_3\delta_3 & s_3\delta_4 \\ 0 & 0 & s_3\delta_3 & c_3\delta_3 & c_3\delta_4 \\ 0 & 0 & s_3\delta_4 & c_3\delta_4 & \alpha_5 \end{bmatrix}, \end{aligned}$$

with $\eta_3 = u_3\hat{v}_3c_3 + \rho_3s_3$.

The sub–block matrices $S_5^{(1)}(1:3, 1:3)$ and $S_5^{(1)}(3:5, 3:5)$ turn out to be symmetric semiseparable.
Let

$$G_2 = \begin{bmatrix} c_2 & s_2 \\ -s_2 & c_2 \end{bmatrix} \text{ such that } G_2 \begin{bmatrix} v_2 \\ \hat{v}_3 \end{bmatrix} = \begin{bmatrix} \hat{v}_2 \\ 0 \end{bmatrix},$$

and

$$\hat{G}_2 = \begin{bmatrix} I_1 & & \\ & G_2 & \\ & & I_2 \end{bmatrix}.$$

Multiplying $\hat{G}_3\hat{S}_5\hat{G}_3^T$ to the left by $\hat{G}_2$ and to the right by $\hat{G}_2^T$, it turns out

$$\begin{aligned} S_5^{(2)} &= \hat{G}_2\hat{G}_3\hat{S}_5\hat{G}_3^T\hat{G}_2^T \\ &= \begin{bmatrix} u_1v_1 & u_1\hat{v}_2 & 0 & 0 & 0 \\ u_1\hat{v}_2 & \eta_2 & s_2\delta_2 & s_2s_3\delta_3 & s_2s_3\delta_4 \\ 0 & s_2\delta_2 & c_2\delta_2 & c_2s_3\delta_3 & c_2s_3\delta_4 \\ 0 & s_2s_3\delta_3 & c_2s_3\delta_3 & c_3\delta_3 & c_3\delta_4 \\ 0 & s_2s_3\delta_4 & c_2s_3\delta_4 & c_3\delta_4 & \alpha_5 \end{bmatrix}, \end{aligned}$$

with

$$\eta_2 = u_2\hat{v}_2c_2 + \rho_2s_2$$

and

$$\begin{bmatrix} \rho_2 \\ \delta_2 \end{bmatrix} \equiv \begin{bmatrix} c_2u_2\hat{v}_3 + s_2\eta_3 \\ -s_2u_2\hat{v}_3 + c_2\eta_3 \end{bmatrix}.$$

Therefore the sub–block matrices $S_5^{(2)}(1:2, 1:2)$ and $S_5^{(2)}(2:5, 2:5)$ are symmetric semiseparable. To end the updating, let us consider the Givens rotation

$$\hat{G}_1 = \begin{bmatrix} G_1 & \\ & I_3 \end{bmatrix},$$

with

$$G_1 = \begin{bmatrix} c_1 & s_1 \\ -s_1 & c_1 \end{bmatrix}$$

such that

$$G_1 \begin{bmatrix} v_1 \\ \hat{v}_2 \end{bmatrix} = \begin{bmatrix} \hat{v}_1 \\ 0 \end{bmatrix}.$$

Then

$$\begin{aligned} S_5^{(3)} &\equiv \hat{G}_1\hat{G}_2\hat{G}_3\hat{S}_5\hat{G}_3^T\hat{G}_2^T\hat{G}_1^T \\ &= \begin{bmatrix} \eta_1 & s_1\delta_1 & s_1s_2\delta_2 & s_1s_2s_3\delta_3 & s_1s_2s_3\delta_4 \\ s_1\delta_1 & c_1\delta_1 & c_1s_2\delta_2 & c_1s_2s_3\delta_3 & c_1s_2s_3\delta_4 \\ s_1s_2\delta_1 & c_1s_2\delta_2 & c_2\delta_2 & c_2s_3\delta_3 & c_2s_3\delta_4 \\ s_1s_2s_3\delta_1 & c_1s_2s_3\delta_3 & c_2s_3\delta_3 & c_3\delta_3 & c_3\delta_4 \\ s_1s_2s_3\delta_4 & c_1s_2s_3\delta_4 & c_2s_3\delta_4 & c_3\delta_4 & \alpha_5 \end{bmatrix} \end{aligned}$$

is symmetric semiseparable with

$$\eta_1 = u_1\hat{v}_1c_1 + \rho_1s_1$$

and

$$\begin{bmatrix} \rho_1 \\ \delta_1 \end{bmatrix} = \begin{bmatrix} c_1u_1\hat{v}_2 + s_1\eta_1 \\ -s_1u_1\hat{v}_2 + c_1\eta_1 \end{bmatrix}.$$

The updating of a symmetric semiseparable matrix of order k has $O(k)$ computational complexity and needs $O(k)$ storage.
Having shown how the semiseparable structure in the matrix (1) can be updated, it turns out quite straightforward how the Lanczos algorithm can be modified in order to compute semiseparable matrices.

Lanczos reduction to semiseparable matrices
Let r_0 be the initial guess, $\beta_0 = \|r_0\|_2$, $q_0 = 0$ and S_0 is the empty matrix.

`for` $i = 1, 2, \ldots$

(a) $q_i = r_{i-1}/\|r_{i-1}\|_2$
(b) $p = Aq_i$
(c) $\alpha_i = q_i^T p$
(d) Compute S_i, i.e., reduce into semiseparable form the augmented matrix

$$\left[\begin{array}{c|c} S_{i-1} & \beta_{i-1}e_{i-1} \\ \hline \beta_{i-1}e_{i-1}^T & \alpha_i \end{array}\right] \text{ with } e_i = [\underbrace{0,\ldots,0}_{i-1},1]^T,$$

(e) $r_i = p - \alpha_i q_i - \beta_{i-1}q_{i-1}$
(f) $\beta_i = \|r_i\|_i$

The step (d) in the Lanczos reduction to semiseparable matrices corresponds to applying one iteration of the QR–method without shift to the matrix S_{i-1} [VAN 05]. This is accomplished applying $i-2$ Givens rotations. Step (d) could be replaced by applying one step of the implicitly shifted QR–method, with the shift chosen in order to improve the convergence of the sequence of the generated semiseparable matrices towards a similar block diagonal one [VAN 04c].
We observe that it is not necessary to compute the product of the Givens rotations at each step. The Givens coefficients are stored in a matrix and the product is computed only when the convergence of the sequence of the semiseparable matrix to a block diagonal form has occurred. As a consequence, the Krylov basis is then updated multiplying Q_k by the latter orthogonal matrix.
The reduction of a symmetric matrix into a similar semiseparable one proposed in this paper has the same properties as the algorithm proposed in [VAN 05]. Therefore, if gaps are present in the spectrum of the original matrix, they are *"revealed"* after some steps of the algorithm [MAS 05]. This property makes the proposed algorithm suitable for computing the largest eigenvalues and the corresponding eigenvectors of sparse or structured matrices, if the large eigenvalues are *"quite well"* separated from the rest of the spectrum. Indeed, the most computationally expensive part, at each step of the proposed algorithm, is a matrix by vector product, and it can be efficiently performed if the matrix is sparse or structured.

III. Numerical experiments

In the previous section, the Lanczos reduction of a symmetric matrix into semiseparable form has been described. The extension to reduce an unsymmetric matrix into an upper triangular semiseparable one, very useful in the applications in order to compute the singular value decomposition, is quite straightforward (for the sake of space, we omit the details of this reduction). The latter algorithm has been considered in the next examples and we will refer to it as `lansvdSS`.
The proposed algorithm has been implemented in `matlab`. To prevent the loss of orthogonality of the Lanczos method [GOL 96, pp. 479–484], the proposed method is based on the implementation of the Lanczos algorithm with partial reorthogonalization [LAR 05], [LAR 98], [SIM 84b] and compared with `lansvd`, an implementation of the Lanczos algorithm with partial reorthogonalization in PROPACK [LAR 05].
Example 1: In this example, we consider a simulated Magnetic Resonance Spectroscopy (MRS) signal derived from an in vivo spectrum measured in the healthy peripheral zone tissue of the prostate [LAU 05]. The discrete simulated signal, made of $N = 256$ data points, was modelled as the sum of $K = 8$ exponentially damped sinusoids (Fig.1),

$$y_n = \sum_{k=1}^{K} a_k e^{j\phi_k(-d_k + j2\pi f_k)t_n}, \quad n = 0,1,\ldots,N-1, \tag{2}$$

with $j = \sqrt{-1}$, a_k the amplitude, ϕ_k the phase, d_k the damping factor, f_k the frequency of the kth sinusoid $k = 1,2,\ldots,K$, K the number of the sinusoids, $t_n = n\Delta t + t_0$ with Δt the sampling interval, t_0 the time between the effective time origin and the first data point. A realistic real-

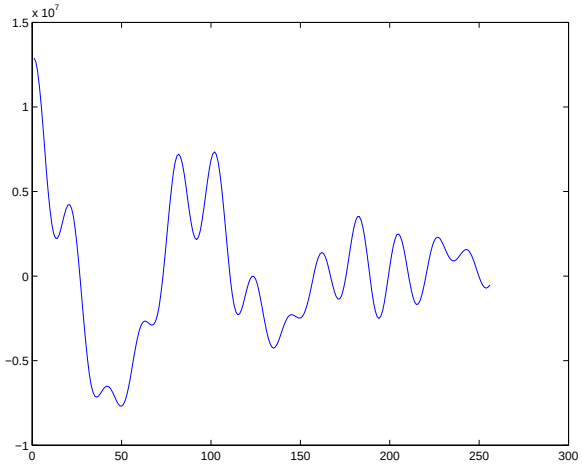


Fig. 1. Original signal (real part).

ization of a noisy signal is obtained adding to the latter signal a white Gaussian noise with zero mean and standard deviation equal to $2.5e+6$ (see Fig.2). An approximation of the original signal is computed by using a state–space method called HLSVD [TUF 82], [LAU 02], [LAU 05], that yields an approximation of the parameters characterizing the signal, i.e., the amplitudes, the phases, the damping factors and the frequencies of the dumped sinusoids in (2). The computationally most intensive part of this method is the computation of the K largest singular values and the corresponding left singular vectors of a Hankel matrix of size $(\lfloor N/2 \rfloor + 1) \times (N - \lfloor N/2 \rfloor)$, whose entries in the first column and last row are the equidistant and consecutive samples of the noisy signal. The approximation of the original signal is then constructed from the K left singular vectors corresponding to the largest K singular values of the Hankel matrix. In Fig.3 the original and

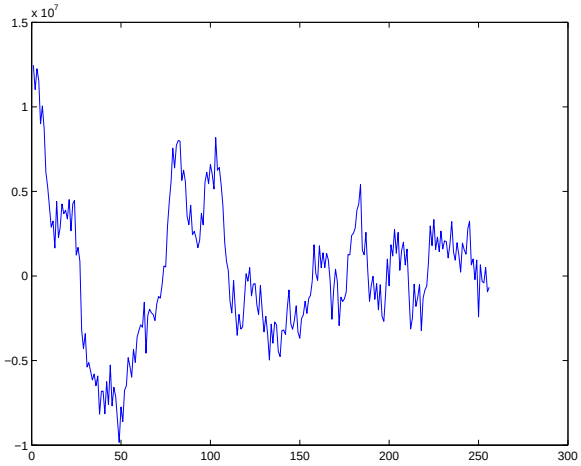


Fig. 2. Noisy signal obtained adding a white Gaussian noise with zero mean and standard deviation equal to $2.5e+6$ (real part).

the reconstructed signals are shown together. Both con-

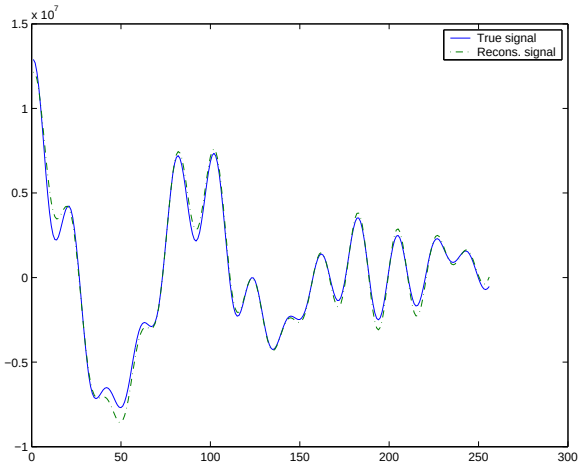


Fig. 3. Original signal (continuous line) vs reconstructed signal by HLSVD (dashed line) (real part).

sidered algorithms, `lansvd` and `lansvdSS`, compute the K largest singular values and the corresponding left singular vectors of the constructed Hankel matrix to full accuracy requiring 17 and 13 steps of the algorithm, respectively. As already described in [VAN 05], [VAN 04b], [MAS 05], the proposed algorithm is very efficient if gaps are present in the distribution of the singular values of the matrix. To show this feature, `lansvdSS` has been used to compute the first $K = 8$ singular values of 7 complex Hankel matrices, whose first row and last column are constructed considering the original signal perturbed by a white Gaussian noise with zero mean and standard deviation $st.dev. = 1e + k, k = 0, 1, \ldots, 6$. The results are depicted in table 1. In the first, second and third column, the level of the standard deviation used to construct the Gaussian noise, the number of steps needed by the proposed algorithm `lansvdSS` to compute the first 8 singular values to full accuracy, and the ratio between the 8th and the 9th singular value, i.e., the gap between the *"signal"* singular values and the *"noise"* singular values, respectively, are reported.

$st.dev.$	$\#steps$	σ_8/σ_9
1	8	$2.0232e+06$
$1e+1$	8	$2.0221e+05$
$1e+2$	8	$1.8447e+04$
$1e+3$	8	$1.9438e+03$
$1e+4$	9	$1.5069e+02$
$1e+5$	10	$2.1517e+01$
$1e+6$	13	$1.7023e+01$

TABLE I
RESULTS OBTAINED COMPUTING THE FIRST 4 SINGULAR VALUES OF 7 COMPLEX HANKEL MATRICES, CONSTRUCTED WITH DIFFERENT LEVELS OF NOISE.

We can observe that the larger the gap, the faster the convergence is to the largest eigenvalues.

Example 2: In this example, the matrix `illc1033.mat` in [SIM 00], of dimension 1033×320, is considered. This matrix has a pronounced gap between the 13th and the 14th singular value (see Fig. 4). The number of steps of the al-

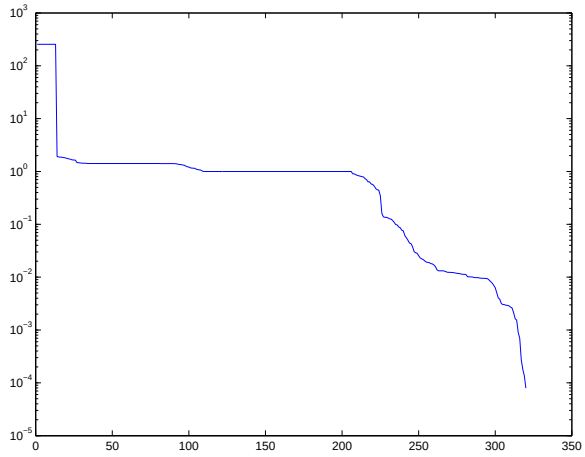


Fig. 4. Distribution of the singular values of the matrix `illc1033.mat` in logarithmic scale.

gorithm `lansvd` in `PROPACK` [LAR 05] to compute the largest 13 singular values of the considered matrix to full accuracy is 53. The proposed algorithm `lansvdSS` requires only 32 steps.

IV. CONCLUSION AND FUTURE WORK.

In this paper, an algorithm that reduces a symmetric matrix into a symmetric semiseparable one is described. The algorithm is based on the Lanczos method. Therefore each iteration relies on the product of the original matrix times a vector. All the developed techniques to prevent the loss of the orthogonality in the Krylov basis (full reorthogonalization, partial reorthogonalization, ...) can be used in this case as well. The extension to reduce a matrix into an upper

semiseparable form to compute the singular value decomposition is quite straightforward. Two numerical examples are considered to show the effectiveness of the proposed method.

Further research will consist of extending the proposed algorithm for computing the rank revealing factorization of sparse and structured matrices.

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