# Lanczos-Type Algorithms for Structured Non-Hermitian Eigenvalue Problems

Roland W. Freund[†]

**Abstract**

The nonsymmetric Lanczos process is a powerful tool for computing a few eigenvalues of large non-Hermitian matrices. Many important applications lead to non-Hermitian matrices that exhibit special structures, such as Hamiltonian or Toeplitz matrices. In this note, we describe variants of the Lanczos process that exploit such special structures.

## 1 The Nonsymmetric Lanczos Process

The nonsymmetric Lanczos process [6] is an iterative procedure that generates a sequence of tridiagonal approximations

$$T_n = \begin{bmatrix} \alpha_1 & \beta_2 & 0 & \cdots & 0 \\ \rho_2 & \alpha_2 & \beta_3 & \ddots & \vdots \\ 0 & \rho_3 & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & \ddots & \beta_n \\ 0 & \cdots & 0 & \rho_n & \alpha_n \end{bmatrix} \in \mathbb{C}^{n\times n}, \quad n = 1, 2, \ldots, \tag{1}$$

to a given matrix $A \in \mathbb{C}^{N\times N}$. The entries of $T_n$ are computed by the following algorithm.

ALGORITHM 1.1 (Lanczos algorithm [6]).

0) Choose $v_1, w_1 \in \mathbb{C}^N$ with $\|v_1\|_2 = \|w_1\|_2 = 1$.
   Set $v_0 = w_0 = 0 \in \mathbb{C}^N$ and $\rho_1 = \eta_1 = \delta_0 = 1$.

For $n = 1, 2, \ldots,$ do:

1) Compute $\delta_n = w_n^T v_n$, $\alpha_n = w_n^T A v_n/\delta_n$, $\beta_n = \eta_n \delta_n/\delta_{n-1}$, $\gamma_n = \rho_n\delta_n/\delta_{n-1}$, and set

$$\tilde{v}_{n+1} = Av_n - v_n\alpha_n - v_{n-1}\beta_n \quad \text{and} \quad \tilde{w}_{n+1} = A^T w_n - w_n\alpha_n - w_{n-1}\gamma_n. \tag{2}$$

2) Compute $\rho_{n+1} = \|\tilde{v}_{n+1}\|_2$ and $\eta_{n+1} = \|\tilde{w}_{n+1}\|_2$.

3) If $\rho_{n+1} = 0$ or $\eta_{n+1} = 0$, then stop.
   Otherwise, set $v_{n+1} = \tilde{v}_{n+1}/\rho_{n+1}$ and $w_{n+1} = \tilde{w}_{n+1}/\eta_{n+1}$.

In addition to the matrices (1), Algorithm 1.1 also produces two sequences of so-called Lanczos vectors $\{v_j\}_{j=1}^n$ and $\{w_j\}_{j=1}^n$, which span the Krylov subspaces $K_n(A, v_1) := \operatorname{span}\{v_1, Av_1, \ldots, A^{n-1}v_1\}$ and $K_n(A^T, w_1) := \operatorname{span}\{w_1, A^T w_1, \ldots, (A^T)^{n-1}w_1\}$, respectively. Furthermore, the Lanczos vectors are biorthogonal, i.e., $w_j^T v_k = 0$ for all $j \neq k = 1, 2, \ldots, n$. We stress that the initial Lanczos vectors $v_1$ and $w_1$ can be chosen as arbitrary unit vectors. The tridiagonal matrix $T_n$ represents a projection of $A$ resulting from

[†]AT&T Bell Laboratories, Room 2C–420, 600 Mountain Avenue, Murray Hill, New Jersey 07974–0636.

an oblique projection process onto $K_n(A, v_1)$ and orthogonally to $K_n(A^T, w_1)$; see, e.g., [7]. This suggests that the eigenvalues of $T_n$ in some sense approximate the spectrum $\sigma(A)$ of $A$. Indeed, $\sigma(T_n)$ typically yields good approximations to some of the eigenvalues of $A$, even for $n \ll N$.

We remark that, in Algorithm 1.1, an exact breakdown or a near-breakdown will occur if $w_n^T v_n \approx 0$. Such breakdowns can be avoided by employing look-ahead techniques; we refer the reader to [2] and the references given there.

## 2 Simplification of the Lanczos Process

As Lanczos already pointed out in [6], Algorithm 1.1 simplifies for Hermitian matrices $A = A^H$ and for complex symmetric matrices $A = A^T$. For $A = A^H$, one chooses $w_1 = \overline{v_1}$ as the complex conjugate of $v_1$, and then $w_n = \overline{v_n}$ for all $n$. Therefore, the second relation in (2) can be deleted, and the resulting Hermitian Lanczos algorithm requires only half the work and storage of Algorithm 1.1. Similarly, if $A = A^T$, one chooses $w_1 = v_1$, and then $w_n = v_n$ for all $n$.

Many important applications lead to matrices $A$ that are neither Hermitian nor complex symmetric, but are $P$-symmetric or $P$-Hermitian in the sense that

$$A^T P = PA, \;\; P = P^T, \quad \text{or} \quad A^H P = PA, \;\; P = P^H, \tag{3}$$

for some nonsingular matrix $P$. For example, if $A$ is a Toeplitz matrix, then the first relation in (3) is satisfied with $P$ being the antidiagonal identity matrix. As a second example, consider real Hamiltonian matrices

$$\mathcal{H} = \begin{bmatrix} F & G \\ H & -F^T \end{bmatrix}, \quad \text{where} \quad F,\; H = H^T,\; G = G^T \in \mathbb{R}^{s \times s}. \tag{4}$$

The eigenvalue problem for real Hamiltonian matrices arises in control theory and also in a number of other applications; see [3] and the references given there. The matrices (4) are characterized by the condition

$$\mathcal{H}^T J = -J\mathcal{H}, \quad \text{where} \quad J := \begin{bmatrix} 0 & I_s \\ -I_s & 0 \end{bmatrix},$$

and hence the scaled Hamiltonian matrix $A = i\mathcal{H}$, $i := \sqrt{-1}$, is $P$-Hermitian with $P := iJ$.

Freund and Zha [5, 1] observed that the nonsymmetric Lanczos process also simplifies for $P$-symmetric and $P$-Hermitian matrices by choosing initial Lanczos vectors $v_1$ and $w_1$ that are coupled by $w_1 = Pv_1/\|Pv_1\|_2$ and $w_1 = \overline{Pv_1}/\|Pv_1\|_2$, respectively. In fact, using (3), one easily verifies that the Lanczos vectors satisfy $w_n = Pv_n/\|Pv_n\|_2$, respectively $w_n = \overline{Pv_n}/\|Pv_n\|_2$, for all $n$. Therefore, the second recurrence relation in (2) can be replaced by essentially a matrix-vector multiplication with $P$. If the computation of such products is cheap (as it is the case for Toeplitz and Hamiltonian matrices), the resulting simplified Lanczos algorithm requires only half the work and storage of Algorithm 1.1.

For the special case of real Hamiltonian matrices (4), the associated simplified Lanczos algorithm was studied in detail by Freund and Mehrmann [3]. In this case, one chooses $v_1$ as a real vector, and then all vectors $v_n$ are real. Together with $P = iJ$, it follows that $w_n = -iJv_n/\|Jv_n\|_2$. Thus the condition $w_n^T v_n = 0$ for an exact breakdown is equivalent to $v_n^T J v_n = 0$, which is always satisfied since $J$ is skew-symmetric. As a consequence, the simplified Lanczos algorithm for Hamiltonian matrices generically performs look-ahead steps of length 2. A sketch of the resulting algorithm is as follows.

ALGORITHM 2.1 (Lanczos algorithm for real Hamiltonian matrices (4) [3]).

0) Choose $v_1 \in \mathbb{R}^{2s}$ with $\|v_1\|_2 = 1$. Set $v_{-1} = v_0 = 0 \in \mathbb{R}^{2s}$ and $\sigma_0 = \rho_1 = 1$.

For $n = 1, 2, \ldots,$ do :

1) Set $\tilde{v}_{2n} = \mathcal{H} v_{2n-1} - v_{2n-1}\xi_n$ and $\rho_{2n} = \|\tilde{v}_{2n}\|_2$.

2) If $\rho_{2n} = 0$, then stop. Otherwise, set $v_{2n} = \tilde{v}_{2n}/\rho_{2n}$.

3) Compute $\sigma_n = v_{2n-1}^T J v_{2n}$, $\beta_n = -v_{2n}^T J \mathcal{H} v_{2n}/\sigma_n$, $\gamma_n = \rho_{2n-1}\sigma_n/\sigma_{n-1}$, and set $\tilde{v}_{2n+1} = \mathcal{H} v_{2n} + v_{2n}\xi_n - v_{2n-1}\beta_n - v_{2n-3}\gamma_n$ and $\rho_{2n+1} = \|\tilde{v}_{2n+1}\|_2$.

4) If $\rho_{2n+1} = 0$, then stop. Otherwise, set $v_{2n+1} = \tilde{v}_{2n+1}/\rho_{2n+1}$.

We note that, in Algorithm 2.1, the coefficients $\xi_n \in \mathbb{R}$ can be chosen arbitrarily, and they can be used to enhance the stability of the recurrences in steps 1) and 3). For a detailed study of Algorithm 2.1, we refer the reader to [3].

## 3 Other Structured Non-Hermitian Matrices

There are also other interesting structured non-Hermitian matrices that are not covered by (3). Numerical calculations in quantum chemistry lead to large symmetric generalized eigenvalue problems $Mx = \lambda Kx$, where $M$ and $K$ are real block matrices of the form

$$M = \begin{bmatrix} B & C \\ C & B \end{bmatrix}, \quad K = \begin{bmatrix} \Sigma & \Lambda \\ -\Lambda & -\Sigma \end{bmatrix}, \quad \text{with} \quad B = B^T,\ C = C^T,\ \Sigma = \Sigma^T,\ \Lambda = -\Lambda^T.$$

Typically, the matrix $K$ is easily invertible, and then the problem reduces to approximating the eigenvalues of the non-Hermitian matrix $A = K^{-1}M$. The matrix $A$ is $K$-symmetric, and thus we can employ the simplified Lanczos algorithm sketched in §2. Furthermore, the eigenvalues of $A$ occur in pairs $\lambda$ and $-\lambda$, and this additional structure can also be exploited by updating coupled pairs of Lanczos vectors rather than single vectors. The resulting Lanczos-type algorithm for the matrices $A = K^{-1}M$ requires only one fourth of the work and storage of Algorithm 1.1; see [4] for a detailed description of this procedure.

Finally, there is an obvious counterpart to (3), namely non-Hermitian matrices $A$ that are $P$-orthogonal or $P$-unitary in the sense that

$$A^T P A = P,\ P = P^T, \quad \text{or} \quad A^H P A = P,\ P = P^H. \tag{5}$$

The structures (5) can also be exploited, and in fact, there is a Lanczos-type algorithm based on Szegő recursions that simplifies for matrices satisfying (5).

## References

[1] R. W. Freund, *Transpose-free quasi-minimal residual methods for non-Hermitian linear systems*, in Recent Advances in Iterative Methods, Springer-Verlag, New York, 1994.

[2] R. W. Freund, M. H. Gutknecht, and N. M. Nachtigal, *An implementation of the look-ahead Lanczos algorithm for non-Hermitian matrices*, SIAM J. Sci. Comput., 14 (1993), pp. 137–158.

[3] R. W. Freund and V. Mehrmann, *A symplectic look-ahead Lanczos algorithm for the Hamiltonian eigenvalue problem*, AT&T Numerical Analysis Manuscript, Bell Laboratories, Murray Hill, NJ, 1994.

[4] R. W. Freund and V. Mehrmann, *A Lanczos-type algorithm for a family of block matrices*, in preparation.

[5] R. W. Freund and H. Zha, *Simplifications of the nonsymmetric Lanczos process and a new algorithm for Hermitian indefinite linear systems*, AT&T Numerical Analysis Manuscript, Bell Laboratories, Murray Hill, NJ, 1994.

[6] C. Lanczos, *An iteration method for the solution of the eigenvalue problem of linear differential and integral operators*, J. Res. Nat. Bur. Standards, 45 (1950), pp. 255–282.
[7] Y. Saad, *Numerical Methods for Large Eigenvalue Problems*, Manchester University Press, Manchester, 1992.