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A LOW-COMPLEXITY DIVIDE-AND-CONQUER METHOD FOR COMPUTING EIGENVALUES AND EIGENVECTORS OF SYMMETRIC BAND MATRICES *

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Abstract.

A framework for an efficient low-complexity divide-and-conquer algorithm for computing eigenvalues and eigenvectors of an $n \times n$ symmetric band matrix with semibandwidth $b \ll n$ is proposed and its arithmetic complexity analyzed. The distinctive feature of the algorithm—after subdivision of the original problem into p subproblems and their solution—is a separation of the eigenvalue and eigenvector computations in the central synthesis problem. The eigenvalues are computed recursively by representing the corresponding symmetric rank $b(p-1)$ modification of a diagonal matrix as a series of rank-one modifications. Each rank-one modification problem can be solved using techniques developed for the tridiagonal divide-and-conquer algorithm. Once the eigenvalues are known, the corresponding eigenvectors can be computed efficiently using modified QR factorizations with restricted column pivoting. It is shown that the complexity of the resulting divide-and-conquer algorithm is $O(n^2b^2)$ (in exact arithmetic).

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Key words: Banded symmetric eigenproblem, divide-and-conquer method, complexity analysis.

1 Introduction.

Given a symmetric band matrix $B \in \mathbb{R}^{n\times n}$ with semibandwidth b (b sub- and superdiagonals, respectively) and no zero entries in the outmost off-diagonals, the problem of computing a spectral decomposition

$$B = V\Lambda V^\top \tag{1.1}$$

with a diagonal eigenvalue matrix $\Lambda = \mathrm{diag}(\lambda_1, \lambda_2, \ldots, \lambda_n)$ and an orthonormal eigenvector matrix $V \in \mathbb{R}^{n\times n}$ is considered.

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The standard approach for solving such a problem is to tridiagonalize B, to compute eigenpairs of the tridiagonal matrix (for example, using the tridiagonal divide-and-conquer method) and then to transform the eigenvectors. It is possible to transform B to tridiagonal form while not enlarging the bandwidth in the process [15]. This obviously improves storage efficiency compared to standard tridiagonalization but can be slower if b is not small enough [14], in part due to unsatisfactory data-locality and a low portion of Level 3 BLAS operations. This motivates attempts to compute (1.1) directly without tridiagonalizing B.

1.1 Related work.

Arbenz, Gander and Golub [2, 3] have developed methods for computing eigenpairs of a low-rank modification of a diagonal matrix. Based on this work, Arbenz [1] has developed a divide-and-conquer method for symmetric band matrices. The arithmetic complexity of that method is $O(n^3)$. Moreover, unsatisfactory numerical accuracy has been observed [1]. Combining divide-and-conquer with inverse iteration improved accuracy but turned out to be less efficient.

The band divide-and-conquer algorithm discussed in this paper differs from Arbenz' algorithm in that it utilizes different approaches for eigenvalue and eigenvector computation. This leads to a significant reduction of the arithmetic complexity. Numerical aspects of the new algorithm will be discussed in a subsequent paper.

The basic steps of the algorithm are described in Section 2, its "core", the computation of eigenpairs of rank-r modifications ($r > 1$) of a diagonal matrix, is discussed in Section 3, and the arithmetic complexity is analyzed in Section 4.

2 A divide-and-conquer algorithm for band matrices.

Three basic steps will be distinguished in the divide-and-conquer method for banded eigenproblems: (i) subdivision, (ii) solution of the subproblems and (iii) synthesis of the solutions of the subproblems.

2.1 Subdivision.

If p is chosen such that

$$n/p \geq b + 1 \tag{2.1}$$

then B can be partitioned into p equally sized blocks of size $n/p \times n/p$ (for simplicity, p is assumed to divide n) according to

$$B = \begin{pmatrix} B_1 & R_1^\top & & & & \\ R_1 & B_2 & R_2^\top & & \mathbf{0} & \\ & R_2 & B_3 & R_3^\top & & \\ & & \ddots & \ddots & \ddots & \\ & \mathbf{0} & & R_{p-2} & B_{p-1} & R_{p-1}^\top \\ & & & & R_{p-1} & B_p \end{pmatrix}. \tag{2.2}$$

The diagonal blocks $B_i \in \mathbb{R}^{n/p \times n/p}$, $i = 1, 2, \ldots, p$, are symmetric and banded with semibandwidth b. The subdiagonal blocks $R_i \in \mathbb{R}^{b \times b}$, $i = 1, 2, \ldots, p-1$, are upper triangular and nonsingular.

For our purpose, the subdiagonal blocks R_i need to be represented as

$$R_i = G_i F_i^\top, \quad i = 1, 2, \ldots, p-1, \tag{2.3}$$

with $F_i, G_i \in \mathbb{R}^{b\times b}$. There is some freedom in choosing these representations. One possibility is to simply choose $G_i = R_i$ and $F_i = I$. Other representations may be favorable for the numerical properties of the algorithm (see also [1]). Details will be discussed in a subsequent paper.

Based on (2.3) the matrices

$$W_i^\top := \left(\mathbf{0}_{b\times(in/p-b)}, F_i^\top, G_i^\top, \mathbf{0}_{b\times((p-i)n/p-b)}\right) \in \mathbb{R}^{b\times n}, \quad i = 1, 2, \ldots, p-1, \tag{2.4}$$

can be constructed. This makes it possible to represent B as a rank-$b(p-1)$ modification of a block diagonal matrix, i.e.,

$$B = \tilde{B} + WW^\top, \tag{2.5}$$

where $\tilde{B} := \operatorname{diag}\left(\tilde{B}_1, \tilde{B}_2, \ldots, \tilde{B}_p\right)$ and $W := (W_1, W_2, \ldots, W_{p-1})$. The matrices $\tilde{B}_i \in \mathbb{R}^{n/p\times n/p}$ are given by

$$\tilde{B}_1 := B_1 - \begin{pmatrix} F_1 \\ \mathbf{0} \end{pmatrix} (F_1^\top, \mathbf{0}), \qquad \tilde{B}_p := B_p - \begin{pmatrix} \mathbf{0} \\ G_{p-1} \end{pmatrix} (\mathbf{0}, G_{p-1}^\top),$$

and, for $i = 2, 3, \ldots, p-1$,

$$\tilde{B}_i := B_i - \begin{pmatrix} \mathbf{0} \\ G_{i-1} \\ \mathbf{0} \end{pmatrix} (\mathbf{0}, G_{i-1}^\top, \mathbf{0}) - \begin{pmatrix} \mathbf{0} \\ F_i \\ \mathbf{0} \end{pmatrix} (\mathbf{0}, F_i^\top, \mathbf{0}).$$

Consequently, they are also symmetric and banded with semibandwidth b.

2.2 Solution of the subproblems.

After having chosen partitioning (2.2) of B and representations (2.3) of R_i, and after having computed $\tilde{B}_i$ from B_i, p banded $n/p \times n/p$ eigendecompositions

$$\tilde{B}_i = \tilde{Q}_i \tilde{\Sigma}_i \tilde{Q}_i^\top, \quad i = 1, 2, \ldots, p, \tag{2.6}$$

are computed using any method for solving symmetric banded eigenproblems (see, for example, [11, 14]).

2.3 Synthesis of the solutions of the subproblems.

Denoting $\tilde{Q} := \operatorname{diag}\left(\tilde{Q}_1, \tilde{Q}_2, \ldots, \tilde{Q}_p\right)$, the matrices

$$U_i^\top = \left(\mathbf{0}_{b\times((i-1)n/p)}, U_{i1}^\top, U_{i2}^\top, \mathbf{0}_{b\times((p-i-1)n/p)}\right), \quad i = 1, 2, \ldots, p-1, \tag{2.7}$$

with $U_{i1}, U_{i2} \in \mathbb{R}^{n/p\times b}$ are computed as

$$U_i := \tilde{Q}^\top W_i \in \mathbb{R}^{n\times b}. \tag{2.8}$$

Combining all the matrices U_i into

$$U := (U_1, U_2, \ldots, U_{p-1}) \in \mathbb{R}^{n \times b(p-1)}$$

and denoting $\tilde{\Sigma} := \operatorname{diag}\left(\tilde{\Sigma}_1, \tilde{\Sigma}_2, \ldots, \tilde{\Sigma}_p\right)$ reveals that B is orthogonally similar to a rank $b(p-1)$ modification of a diagonal matrix,

$$B = \tilde{Q}(\tilde{\Sigma} + UU^\top)\tilde{Q}^\top. \tag{2.9}$$

Consequently, the central task of the band divide-and-conquer algorithm is the solution of the *synthesis problem*, that is, the eigenanalysis of the *synthesis matrix*

$$S := \tilde{\Sigma} + UU^\top = \tilde{\Sigma} + \sum_{i=1}^{p-1} U_i U_i^\top, \tag{2.10}$$

a symmetric modification of a diagonal matrix. $U \in \mathbb{R}^{n \times b(p-1)}$ is not necessarily of low rank since $b(p-1) \leq n$.

3 Solution of the synthesis problem.

In the algorithm proposed for computing a spectral decomposition

$$S = Q\Sigma Q^\top, \tag{3.1}$$

the eigenvalues of S are computed first (see Section 3.1) and then, using this information, the required eigenvectors are established (see Section 3.2).

It follows from (2.9), (2.10), and (3.1) that

$$B = \tilde{Q}Q\ \Sigma\ Q^\top\tilde{Q}^\top \quad \text{and thus} \quad \sigma(\Lambda) = \sigma(\Sigma).$$

An orthogonal set of eigenvectors of B can be found as the product

$$V := \tilde{Q}Q. \tag{3.2}$$

3.1 The eigenvalues of the synthesis matrix.

For simplicity it is assumed that p is a power of two, that is, $p = 2^q$. This is not a severe restriction of generality. Even if this assumption is not satisfied, all steps can be carried out analogously after a slightly modified first step.

Arbenz, Gander, and Golub [2, 3] developed a "$1 \times r$ approach" for computing eigenpairs of a rank r modification of a diagonal matrix, that is, their method essentially transforms the problem into an $r \times r$ problem. It will become clear in Section 4 why a different approach is taken in this paper. For the eigenvalue computation the problem is broken up into a sequence of rank-one modifications, enabling the use of all the technology developed for the tridiagonal divide-and-conquer method, for example, the stabilization [12]. A crucial difference, however, is that the eigenvectors are *not* accumulated in this process in order to avoid the corresponding $O(n^3)$ effort (see Section 3.2).

The computation of the eigenvalues of S is based on the following observations.

- Due to the sparsity structure of the matrices U_i (see (2.7)) the eigenvalues of the matrices

$$\begin{pmatrix} \tilde{\Sigma}_i & \\ & \tilde{\Sigma}_{i+1} \end{pmatrix} + \begin{pmatrix} U_{i1} \\ U_{i2} \end{pmatrix} (U_{i1}^\top, U_{i2}^\top)$$

and

$$\begin{pmatrix} \tilde{\Sigma}_{i+2} & \\ & \tilde{\Sigma}_{i+3} \end{pmatrix} + \begin{pmatrix} U_{i+2,1} \\ U_{i+2,2} \end{pmatrix} (U_{i+2,1}^\top, U_{i+2,2}^\top)$$

can be computed independently (in parallel) based on the representation

$$S = \tilde{\Sigma} + \sum_{i=1}^{p/2} U_{2i-1} U_{2i-1}^\top + \sum_{i=1}^{p/4} U_{4i-2} U_{4i-2}^\top + \sum_{i=1}^{p/8} U_{8i-4} U_{8i-4}^\top + \cdots + U_{p/2} U_{p/2}^\top.$$

Thus, the rank $b(p-1)$ modification problem (2.10) can be solved as a series of $p-1$ modification problems of rank b.

- The eigenvalues of every rank b modification can be computed from a series of rank-one modifications (using the "$b \times 1$ approach" of [9]).

- A hybrid form between the "$1 \times b$ approach" developed by Arbenz, Gander and Golub, and the "$b \times 1$" approach, a "$b/k \times k$ approach" with $1 < k < b$ (suggested by G. H. Golub) remains to be investigated.

The eigenvalue computations have the structure of a binary tree of depth $q = \log_2(p)$ with levels $l = 1, 2, \ldots, q$. The p blocks $\tilde{B}_1, \tilde{B}_2, \ldots, \tilde{B}_p$ are the leaves at the bottom level $l = q$. The desired eigenvalues of S are computed at the top level ($l = 1$), that is, in the root of the tree. At each level l of the tree, eigenvalues as well as eigenvectors of 2^{l-1} rank b synthesis problems are computed but the eigenvector information is not accumulated from one level to the next. All rank b synthesis problems of each level can be solved in parallel, independently of each other.

It suffices to illustrate this strategy for the case $p = 8$:

$$\tilde{\Sigma} + \sum_{i=1}^{7} U_i U_i^\top = \tilde{\Sigma} + \sum_{i=1}^{4} U_{2i-1} U_{2i-1}^\top + \sum_{i=1}^{2} U_{4i-2} U_{4i-2}^\top + U_4 U_4^\top.$$

The eigenvalues and eigenvectors of

$$\begin{pmatrix} \tilde{\Sigma}_1 & \\ & \tilde{\Sigma}_2 \end{pmatrix} + \begin{pmatrix} U_{11} \\ U_{12} \end{pmatrix} \begin{pmatrix} U_{11} \\ U_{12} \end{pmatrix}^\top, \qquad \begin{pmatrix} \tilde{\Sigma}_3 & \\ & \tilde{\Sigma}_4 \end{pmatrix} + \begin{pmatrix} U_{31} \\ U_{32} \end{pmatrix} \begin{pmatrix} U_{31} \\ U_{32} \end{pmatrix}^\top,$$

$$\begin{pmatrix} \tilde{\Sigma}_5 & \\ & \tilde{\Sigma}_6 \end{pmatrix} + \begin{pmatrix} U_{51} \\ U_{52} \end{pmatrix} \begin{pmatrix} U_{51} \\ U_{52} \end{pmatrix}^\top, \qquad \begin{pmatrix} \tilde{\Sigma}_7 & \\ & \tilde{\Sigma}_8 \end{pmatrix} + \begin{pmatrix} U_{71} \\ U_{72} \end{pmatrix} \begin{pmatrix} U_{71} \\ U_{72} \end{pmatrix}^\top$$

can be computed independently at the bottom level $l = 3$. Parts of the respective eigenvector matrices are used to obtain $\tilde{U}_2$ from U_2, $\tilde{U}_4$ from U_4 and $\tilde{U}_6$ from U_6. Then the eigenvalues and eigenvectors of

$$\begin{pmatrix} \tilde{\Sigma}'_1 & \\ & \tilde{\Sigma}'_2 \end{pmatrix} + \begin{pmatrix} \tilde{U}_{21} \\ \tilde{U}_{22} \end{pmatrix} \begin{pmatrix} \tilde{U}_{21} \\ \tilde{U}_{22} \end{pmatrix}^\top \quad \text{and} \quad \begin{pmatrix} \tilde{\Sigma}'_3 & \\ & \tilde{\Sigma}'_4 \end{pmatrix} + \begin{pmatrix} \tilde{U}_{61} \\ \tilde{U}_{62} \end{pmatrix} \begin{pmatrix} \tilde{U}_{61} \\ \tilde{U}_{62} \end{pmatrix}^\top$$

can be computed independently at the next level $l = 2$. At the top level $l = 1$, parts of the computed eigenvector matrices are used to obtain $\tilde{U}'_4$ from $\tilde{U}_4$. Finally, *only* the eigen*values* of

$$\begin{pmatrix} \tilde{\Sigma}''_1 & \\ & \tilde{\Sigma}''_2 \end{pmatrix} + \tilde{U}'_4 \tilde{U}'^\top_4$$

are computed. They are obviously identical to those of the matrix S.

The intermediate eigenvector matrices are not accumulated. Only their first or last $2^i n/p$ rows are required at level $q - i$ for updating the remaining modification matrices. There are two crucial differences to the "classical" divide-and-conquer algorithm for tridiagonal matrices ([6, 8, 13]): In the tridiagonal case (i) each synthesis problem is only a rank-*one* modification problem, and (ii) the final eigenvector matrix V is computed by accumulating (multiplying) the intermediate eigenvector matrices at every level, leading to an overall arithmetic complexity of $O(n^3)$ in the worst case [7].

3.2 The eigenvectors of the synthesis matrix.

Essential for the reduction of the cubic to a quadratic complexity in n is a different approach for computing the eigenvectors of S. The basic idea is to take advantage of the eigenvalues σ_i already computed and to find an efficient way for computing bases of the null spaces of the matrices $S - \sigma_i I$.

Alternatively, when its eigenvalues σ_i are available, the eigenvectors of S could be computed using the method developed by Arbenz et al. [2, 3], also described in [9]. This approach involves matrices of the form $U^\top(\tilde{\Sigma} - \sigma_i I)^{-1}U$. It is very attractive if S is a *low rank* modification of a diagonal matrix, that is, if U has significantly fewer than n columns, because in this case it leads to a reduction of the problem size.

In the divide-and-conquer algorithm described in this paper, however, the situation is different. It is shown in Section 4 that the optimum choice of the parameter p in terms of arithmetic complexity implies that S is a *high rank* modification of a diagonal matrix (see Section 4.2). In particular, the matrices $U^\top U$ and $UU^\top$ are about the *same* size! Therefore, it turns out to be preferable to compute the eigenvectors of S "directly" (from their definition) as bases of the null spaces of the matrices $S - \sigma_i I$.

The key observation is that $UU^\top$ and therefore $S - \sigma_i I$ is a *block-tridiagonal* matrix. A very efficient way of finding a basis for its null space which minimizes fill-in and therefore preserves the favorable structure is to perform a modified QR factorization with *restricted column pivoting*, very similar to the method suggested by Bischof et al. (see, for example, [4, 5]): QR factorizations are computed block-column wise, and pivoting is restricted to each block-column of width n/p. In exact

arithmetic, this yields a rank-revealing factorization with a "step matrix" whose upper bandwidth is at most $3n/p$. Its null space has a simple block structure which can be expressed explicitly and computed very efficiently based on a recursion which involves the solution of nonsingular triangular $n/p \times n/p$ linear systems. This method will be described in more detail in a forthcoming paper.

4 The arithmetic complexity.

In the following complexity analyses of the divide-and-conquer algorithm outlined in Sections 2 and 3 floating-point additions, subtractions, multiplications and divisions are counted. Only the asymptotically dominating terms of the exact flop counts are considered. It should be emphasized that under the assumptions stated at the beginning of Section 1 the multiplicity of each eigenvalue of S cannot exceed b. More general situations will be studied in a forthcoming paper.

So far, the subdivision parameter $p = p(n, b)$ has not been determined. It is shown in this section that

$$p = O\left(\frac{n}{b}\right) \quad \text{with} \quad p \leq \frac{n}{b+1}$$

is optimal in terms of the arithmetic complexity of the algorithm proposed.

4.1 Operation counts.

Count 1: Computation of the factorizations (2.3) requires at most

$$(8/3)(p-1)b^3 \quad \text{flops.}$$

Count 2: Computation of the p band matrices $\tilde{B}_1, \ldots, \tilde{B}_p$ requires at most

$$4(p-1)b^3 \quad \text{flops.}$$

Count 3: Computation of the eigendecompositions (2.6) of the p symmetric $n/p \times n/p$ band matrices $\tilde{B}_i$ in the solution step requires at most

$$(14/3)(n^3/p^2) + O(n^2/p) \quad \text{flops.}$$

This is an overestimation because it counts the flops required for tridiagonalizing a *full* symmetric matrix and explicitly computing the transformation matrix ([11], p. 415), followed by backtransforming the eigenvectors.

Count 4: Computation (2.8) of the matrices $U_1, U_2, \ldots, U_{p-1} \in \mathbb{R}^{n \times b}$ to establish the central rank $b(p-1)$ synthesis problem (2.9) requires

$$(p-1)\left((2b + 2b - 1)\, b\, \frac{n}{p}\right) = n\, \frac{p-1}{p}\, b(4b-1) < 4nb^2 \quad \text{flops.}$$

Count 5: Computation of all the eigenvalues of the synthesis matrix S, which coincide with the desired eigenvalues Λ of B, requires a series of eigenanalyses of rank b modification problems. Each of these can, in turn, be analyzed as a series of rank-one modification problems as described in Section 3.1. The corresponding flop counts are as follows (details can be found in [10]):

- The eigenanalysis of a rank-one modification problem $D + xx^\top \in \mathbb{R}^{n\times n}$ requires at most $4n^2(m + 2e + 2) + 5n - 2$ flops. This count assumes a floating-point arithmetic $\mathbb{F}(2, m, e_{\min}, e_{\max})$, where m denotes the length of the mantissa, $e_{\min}$ is the smallest exponent, $e_{\max}$ the largest one, $e := e_{\max} + 1$, and that standard bisection is used for locating each eigenvalue. It considers a worst-case scenario where no deflation (see [8]) occurs and also includes the Gu/Eisenstat corrections [12] for numerical stability.
- A complete eigenanalysis of a rank b modification problem $\Sigma + U_i U_i^\top$ where $U_i \in \mathbb{R}^{n\times b}$ requires at most $O(n^2b^2) + O(nb^3)$ flops using the technique mentioned in Section 3.2 for computing the eigenvectors.
- The actual computation of the eigenvalues of S proceeds in a tree structure with q levels where $q = \lfloor \log_2 p \rfloor$. At each level complete eigenanalyses of rank b modifications of diagonal matrices are required (see Section 3.1), which lead to a total count of at most

$$O(n^2b^2) + O(nb^3 \log_2 p) + O(nb^3) \quad \text{flops.}$$

Count 6: Computation of orthogonal eigenvectors Q of S proceeds in several steps (details will be described in a forthcoming paper).

Step 1: Computation of all block-tridiagonal matrices $\tilde{\Sigma} + UU^\top - \sigma_i I$ requires less than $6n^2b/p + n^2 + n$ flops.

Step 2: Computation of each modified QR factorization

$$\tilde{\Sigma} + UU^\top - \sigma_i I = Q_i M_i$$

with restricted column pivoting to limit fill-in can be performed in at most $O(n^3/p^2)$ flops. Consequently, for all different σ_i this computation requires at most $O(n^4/p^2)$ flops.

Step 3: Computation of the null spaces X_i of the matrices M_i for all different σ_i can be performed with at most $O(n^4/p^2)$ flops.

Step 4: Orthonormalization within the eigenvector matrices X_i requires $O(n^2b)$ flops. Eigenvectors corresponding to distinct eigenvalues are orthogonal.

For given eigenvalues σ_i of $\tilde{\Sigma}+UU^\top$ corresponding eigenvectors Q can therefore be computed with

$$O(n^4/p^2) + O(n^2b) \quad \text{flops.}$$

Count 7: The final computation of the eigenvectors V of B according to (3.2) requires at most

$$2n^3/p \quad \text{flops}$$

because of the block-diagonal structure of $\tilde{Q}$ (see Section 2.3).

4.2 The total arithmetic complexity.

The summarized flop counts for Steps 1–7 are

Count 1: $O(pb^3)$ **Count 2:** $O(pb^3)$
Count 3: $O(n^3/p^2) + O(n^2/p)$ **Count 4:** $O(nb^2)$
Count 5: $O(n^2b^2) + O(nb^3 \log_2 p) + O(nb^3)$ **Count 6:** $O(n^4/p^2) + O(n^2b)$
Count 7: $O(n^3/p)$.

The optimum choice of p is found as

$$p = O\left(\frac{n}{b}\right) \tag{4.1}$$

subject to condition (2.1). Note that (4.1) implies $b(p-1) = O(n)$ which makes the synthesis matrix (2.10) a *high-rank* modification of a diagonal matrix (as already mentioned in Section 3.2).

For this choice of p the corresponding total arithmetic complexity of the algorithm described in Sections 2 and 3 is

$$O(n^2b^2) \quad \text{flops.}$$

5 Conclusion.

A new divide-and-conquer algorithm for computing eigenvalues and eigenvectors of an $n \times n$ symmetric band matrix B with semibandwidth b has been described.

A very attractive feature of this algorithm is its low arithmetic complexity of $O(n^2b^2)$ floating-point operations for $b \ll n$. If applied to symmetric tridiagonal eigenproblems ($b = 1$) this algorithm is of quadratic complexity. This is a significant advantage over the well-known standard divide-and-conquer method for symmetric tridiagonal eigenproblems [6, 8, 13], which can be of cubic order in the worst case.

The algorithm developed is expected to be highly efficient, sequentially as well as in parallel. Its numerical properties are currently being investigated and an implementation will be available soon.

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