A NEW HYBRID PROCEDURE FOR COMPUTING EIGENVECTORS OF TRIDIAGONAL SYMMETRIC UNREDUCED MATRICES

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We present a new hybrid procedure for computing accurate approximations of eigenvectors of tridiagonal symmetric unreduced matrices based on the algorithm proposed by S.K.Godunov et al. [2] and Inverse Iteration. The new method uses very accurate shifts that do not break down Inverse Iteration and does not require reorthogonalization of the eigenvectors corresponding to clustered eigenvalues, reducing Inverse Iteration complexity in the worst case from $O(n^3)$ to $O(n^2)$ floating point operations. At the same time the new procedure allows to achieve iterative improvement over the ordinary Godunov's procedure, which is not guaranteed to produce accurate solutions in the absence of directed rounding mechanism.

1. Introduction

Construction of algorithms that allow to solve symmetric tridiagonal eigenvalue problem using $O(n^2)$ floating point operations with guaranteed accuracy has become one of the most pressing problems of the modern computer algebra. Indeed, QR method, one of the most accurate methods for solving eigenvalue problems, requires $6n^3$ arithmetic operations and $O(n^2)$ square roots operations [1] when eigenvectors of a tridiagonal matrix are desired. It is well known that Inverse Iteration procedure takes $O(n^2)$ operations to find eigenvectors, corresponding to well separated eigenvalues. To achieve numerical orthogonality of the eigenvectors corresponding to clustered eigenvalues, reorthogonilization procedures, such as Modified Gram-Schmidt process, should be applied in the Inverse Iteration, increasing algorithm complexity to $O(n^3)$ operations. In the case of clustered eigenvalues Divide-and-Conquer algorithm requires much fewer than $O(n^3)$ operations due to the deflation process.

Recently there have been attempts to construct hybrid procedures based on the Divide-and-Conquer and Inverse Iteration methods. In 1997 Inderjit Dhillon proposed a new $O(n^2)$ algorithm for the symmetric tridiagonal eigen-problem based on the LDL^T factorizations and Inverse Iteration, although without the formal proof of the correctness of the algorithm. Much earlier, in 1985, S.K. Godunov, B.I.Kostin and A.D.Mitchenko [3] proposed a Sturm sequence based method (algorithm 1) that allows to determine all eigenvectors of tridiagonal symmetric matrices with guaranteed accuracy using $11n^2$ floating point operations. The algorithm gives provably accurate solutions to symmetric tridiagonal problems on the architectures with extended precision and directed rounding [2]. In the absence of directed rounding, results delivered by the method do not have guaranteed nature, and are not as accurate as some Inverse Iteration implementations (see section 3).

In the paper we present a new procedure for computing eigenvectors of symmetric tridiagonal unreduced matrices based on the Godunov's method and Inverse Iteration method. In the absence of directed rounding and extended precision, eigenvectors, computed according to the Godunov's algorithm, are nearly orthogonal to machine precision and can be used as very accurate starting vectors in the Inverse Iteration, insuring convergence to the desired accuracy in a few steps. Near orthogonality of the starting eigenvectors eliminates the need for the reorhogonalization of the eigenvectors corresponding to closely clustered eigenvalues, reducing complexity of the hybrid Godunov – Inverse Iteration procedure to $O(n^2)$ arithmetic operations with floating point. Throughout the paper we assume that symmetric matrices with arbitrary structure can be reduced to tridiagonal form with orthogonal transformations, which preserve spectral properties of original matrices to machine precision.

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2. Godunov - Inverse Iteration Procedure

Consider eigenvalue problem for a tridiagonal symmetric matrix T in the Euclidean subspace $R^{n\times n}$. The problem consists in finding non-zero vectors $x_i \in R^n$ and numbers $\lambda_i \in R$ that satisfy the following equation:

$$Tx_i = \lambda_i x_i, \ _{i=1,\ldots,n}. \tag{1}$$

When the matrix T is unreduced, i.e. does not have zero entries among the codiagonal elements, its eigenvalues λ_i are distinct, while eigenvectors x_i are unique up to a scale factor and form an orthogonal basis in $R^{n\times n}$ [4].

All eigenvalues of the matrix T can be found by the bisection algorithm, in $O(bn^2)$ operations, where b is the number of bits of precision in a computer representation of floating point numbers [1]. We apply bisection algorithm [2] to compute intervals (a_i, b_i) containing eigenvalues λ_i computed with guaranteed accuracy:

$$|b_i - a_i| \le \epsilon_{mach}\|T\|_\infty, \ _{i=1,\ldots,n}, \tag{2}$$

where ϵ_{mach} is the unit roundoff error. In the Godunov's method eigen-interval bounds a_i and b_i are used to compute left- and right-hand-side Sturm sequences $P_0^+, \ldots P_{n-1}^+$ and $P_0^-, \ldots P_{n-1}^-$ from the minors corresponding to the operators $T - a_i I$ and $T - b_i I$ respectively [3]. Here I is $n \times n$ identity matrix. Then the sequences are combined into the compound Sturm sequence, which is used to compute eigenvector approximation x_i, corresponding to the eigenvalue $\lambda_i \in (a_i, b_i)$. We give the detailed description of the procedure below. Note that the complexity of the method is $11n$ operations per an eigenvector.

Algorithm 1 (Godunov's Method). *Compute approximate eigenvector U of the tridiagonal matrix $T = T^T \in R^{n\times n}$ with main diagonal d and codiagonal b, corresponding to the eigenvalue $z \in (x, y)$ s.t. $|y - x| \le \epsilon_{mach}\ \|T\|_\infty$, where ϵ_{mach} is machine precision.*

godunov_eigenvector((x, y), d, b)

$P_0^+ = |b_0|/(d_0 - y)$
if $(P_0^+ \le 0)$ $M_0 = 1$
else $M_0 = 0$
for $i = 1 : n-2$
  $P_i^+ = |b_i|/(d_i - y - |b_{i-1}|) \cdot P_{i-1}^+$
  if $(P_i^+ \le 0)$ $M_i = M_{i-1} + 1$
  else $M_i = M_{i-1}$
end
$P_{n-1}^+ = 1/(d_{n-1} - y - |b_{n-2}|) \cdot P_{n-2}^+$
if $(P_{n-1}^+ \le 0)$ $M_{n-1} = M_{n-2} + 1$
else $M_{n-1} = M_{n-2}$
$P_{n-1}^- = d_{n-1} - x$
if $(P_{n-1}^- \le 0)$ $L_{n-1} = n - 1$
else $L_{n-1} = 0$
for $k = n-2 : 1, k--$
  $P_k^- = (d_k - x - |b_k|/P_{k+1}^-)/|b_{k-1}|$
  if $(P_k^- \le 0)$ $L_k = L_{k+1} - 1$
  else $L_k = L_{k+1}$
  if $(M_k == L_{k+1} \bigcap (P_{k-1}^+ - P_k^-) \cdot (1/P_{k+1}^- - 1/P_k^+) \le 0)$ *break*
end
$Ctg = \{P_0^+, P_1^+, \ldots, P_{k-1}^+, P_k^-, P_{k+1}^-, \ldots, P_{n-1}^-\}$
$U_0 = 1$

for $i = 0 : n-1, i++$
$U_i = U_{i-1} \cdot -sign(b_{i-1})/Ctg_{i-1}$
end
return $U/\|U\|$
end

On architectures with extended precision and directed rounding, eigenvectors x_i are provably accurate and the following error estimate holds [3]:

$$\|(T - \lambda_i I)x_i\|_2 \leq 13\sqrt{3}\epsilon_{mach}\|T\|_\infty. \tag{3}$$

Here again I denotes $n \times n$ identity matrix and ϵ_{mach} is the unit roundoff error. Eigenvectors, computed according to the algorithm (1) on the architectures with IEEE double precision without directed rounding, belong to some close vicinity of the eigenvector x_i, having nontrivial component in the direction of the desired eigenvector. We propose to use such an eigenvector as a starting vector x_i^0 in the Inverse Iteration procedure:

$$(T - \tilde{\lambda}_i I)x_i^{k+1} = \tau x_i^k, \ _{k=0,1,2,\ldots} \tag{4}$$

where $\|x_i^k\| = 1$ and the scalar τ is chosen to make $\|x_i^{k+1}\| = 1$. When the starting eigenvector x_i^0 is not chosen deterministically, for instance in the LAPACK version of the algorithm x_i^0 is a random vector from the Uniform distribution on $(-1, 1)$, reorthogonalization procedure is incorporated into the Inverse Iteration. This is necessary to maintain orthogonality among the eigenvectors corresponding to clustered eigenvalues. Being almost orthogonal to machine precision ϵ_{mach}, starting eigenvector x_i^0, computed according to the Godunov's method, does not require additional reorthogonilization, what allows to eliminate Modified Gram-Schmidt procedure from the Inverse Iteration.

When the shift $\tilde{\lambda}_i$ in (4) is too close to the actual eigenvalue λ_i, the operator $T - \tilde{\lambda}_i I$ is almost singular and the iteration breaks down. Such situations are illustrated in the tables 4 and 6 where in the LAPACK and EISPACK versions of the Inverse Iteration some eigenvectors failed to converge and as the result orthogonality-loss measure $\|X^T X - I\|_F$ was unacceptable. Instead of the eigenvalue approximation $\tilde{\lambda}_i = (a_i + b_i)/2$ we use right boundary of the eigen-interval (a_i, b_i) as the shift $\tilde{\lambda}_i = b_i$ to avoid overflow in the computation. The new procedure is formally described by the following algorithm:

Algorithm 2 (Godunov - Inverse Iteration Method). *Compute eigenvectors x_i, $i = 1, \ldots, n$ of the tridiagonal matrix $T = T^T \in R^{n \times n}$ with main diagonal d and codiagonal b, corresponding to the eigenvalues $\lambda_i \in (\alpha_i, \beta_i), i = 1, \ldots, n$ s.t. $|\beta_i - \alpha_i| \leq \epsilon_{mach} \ \|T\|_\infty$, where ϵ_{mach} is machine precision.*

godunov_inverse_iteration((α_i, β_i), **d, b**)
for $(i = 0, i < n, i++)$
$k = 0$
$\delta = 13\sqrt{3}\ \epsilon_{mach}$
$x_i^0 =$ **godunov_eigenvector**$((\alpha, \beta), \mathbf{d}, \mathbf{b})$
$\gamma_i = \beta_i$
if $(k > 0 \cap |\gamma_i - \gamma_{i-1}| \leq 10\ \epsilon_{mach}\ |\gamma_i|)$
then $\gamma_i = \gamma_{i-1} + 10\epsilon_{mach}|\gamma_i|$
do
Factor $(T - \gamma_i I) = LDL^T$
Solve $LDL^T z^{k+1} = x_i^k$
$x_i^{k+1} = z^{k+1}/\|x_i^{k+1}\|_2$
$k = k + 1$
while $(\|(T - \beta I)z^{k+1}\|_\infty > \delta\|T\|_\infty)$
end

3. Testing Results

We implemented and tested algorithms 1 and 2 as well as LAPACK and EISPACK versions of the Inverse Iteration algorithm [1] in ANSI C, using IEEE double precision (GNU C compiler) on a Pentium II processor. We used Bisection method to compute eigen-intervals (a_i, b_i) with the accuracy $|b_i - a_i| \le \epsilon_{mach}\|T\|_\infty$. Intervals (a_i, b_i) were used in the original Godunov's method and in the new Godunov – Inverse Iteration procedure, while in the LAPACK and EISPACK versions of the Inverse Iteration we used $\tilde{\lambda}_i = (a_i + b_i)/2$ as the eigenvalue approximations. In all of the tests presented below Godunov – Inverse Iteration procedure converged to desired accuracy in just one step, while the results are at least as good as in the LAPACK and EISPACK versions of the algorithm, at the same time we get a significant improvement over the original Godunov's algorithm. Note that the new procedure, as well as the Godunov's algorithm are very robust procedures, and do not break down when eigenvalues used in the computations are very accurate.

Example 1. $n = 24,\ S = \{S_{ij}\},\ i, j = 0, 1, \ldots, n-1$

$$S_{ij} = \begin{cases} 0, & i = j \\ (i+2)/\sqrt{4(i+2)^2 - 1}, & |i-j| \le 1 \end{cases}$$

$\max\|\tilde{\lambda}_k(S) - \lambda_k(S)\| = 2.7755575615628914e-16,\ k = 1, \ldots, n$		
	$\max\|(S - \lambda_k I)x_k\|_2$	$\|X^T X - I\|_F$
Godunov Method	$7.3513184540692025e-15$	$6.0095114958263332e-14$
EISPACK Inverse Iteration	$2.0467254147379373e-14$	$1.8633084865971006e-13$
LAPACK Inverse Iteration	$2.5382219767164785e-16$	$1.9096045938831537e-15$
Godunov - Inverse Iteration	$2.5602944862447319e-16$	$2.3784234169765855e-15$

Table 1. Error estimates of the eigenvectors $X = |x_k|_{k=1,\ldots,n}$ of S, corresponding to eigenvalues $\tilde{\lambda}$ computed with maximum absolute deviation $\Delta = 2.7755575615628914e-16$ from the exact eigenvalues λ.

$\max\|\tilde{\lambda}_k(S) - \lambda_k(S)\| = 1.1102230246251565e-16,\ k = 1, \ldots, n$		
	$\max\|(S - \lambda_k I)x_k\|_2$	$\|X^T X - I\|_F$
Godunov Method	$4.8688756855745829e-15$	$3.1930538735098823e-14$
EISPACK Inverse Iteration	$1.4142897691197826e-14$	$9.7529023714049282e-14$
LAPACK Inverse Iteration	$1.2656964587626072e-16$	$1.9059052297984708e-15$
Godunov - Inverse Iteration	$1.3115747911312276e-16$	$1.8111076211312865e-15$

Table 2. Error estimates of the eigenvectors $X = |x_k|_{k=1,\ldots,n}$ of S, corresponding to eigenvalues $\tilde{\lambda}$ computed with maximum absolute deviation $\Delta = 1.1102230246251565e-16$ from the exact eigenvalues λ.

Example 2. $n = 100$

$$Q = \begin{pmatrix} 2 & -1 & & \cdots & 0 \\ -1 & 2 & \ddots & & \vdots \\ & \ddots & \ddots & \ddots & \\ \vdots & & \ddots & 2 & -1 \\ 0 & \cdots & & -1 & 2 \end{pmatrix} \tag{5}$$

Example 3. $n = 100$

$$R = \begin{pmatrix} 0 & 0.5 & & \cdots & 0 \\ 0.5 & 0 & \ddots & & \vdots \\ & \ddots & \ddots & \ddots & \\ \vdots & & \ddots & \ddots & 0.5 \\ 0 & \cdots & & 0.5 & 0 \end{pmatrix} \tag{6}$$

$\max\lvert\tilde{\lambda_k}(Q) - \lambda_k(Q)\rvert = 1.3322676295501878e-15,\ k = 1,\ldots,n$		
	$\max\lVert(Q-\lambda_k I)x_k\rVert_2$	$\lVert X^T X - I\rVert_F$
Godunov Method	$9.1865709358232547e-13$	$6.5674740690484012e-12$
EISPACK Inverse Iteration	$1.5972031730641600e-13$	$5.3111542229596125e-12$
LAPACK Inverse Iteration	$9.0534322991756901e-16$	$1.2304642238924916e-14$
Godunov - Inverse Iteration	$9.0483549862370509e-16$	$1.3787143826091051e-14$

Table 3. Error estimates of the eigenvectors $X = |x_k|_{k=1,\ldots,n}$ of Q, corresponding to eigenvalues $\tilde{\lambda}$ computed with maximum absolute deviation $\Delta = 1.3322676295501878e-15$ from the exact eigenvalues λ.

$\max\lvert\tilde{\lambda_k}(Q) - \lambda_k(Q)\rvert = 8.8817841970012523e-16,\ k = 1,\ldots,n$		
	$\max\lVert(Q-\lambda_k I)x_k\rVert_2$	$\lVert X^T X - I\rVert_F$
Godunov Method	$4.0409590033451748e-13$	$3.2089258554650916e-12$
EISPACK Inverse Iteration	$3.5660764663933954e-13$	$1.0000000000000000e+00$
LAPACK Inverse Iteration	$4.7201413487856058e-16$	$1.0000000000000000e+00$
Godunov - Inverse Iteration	$4.7342893020488205e-16$	$1.1064736864164124e-14$

Table 4. Error estimates of the eigenvectors $X = |x_k|_{k=1,\ldots,n}$ of Q, corresponding to eigenvalues $\tilde{\lambda}$ computed with maximum absolute deviation $\Delta = 8.8817841970012523e-16$ from the exact eigenvalues λ.

$\max\lvert\tilde{\lambda_k}(R) - \lambda_k(R)\rvert = 4.4408920985006262e-16,\ k = 1,\ldots,n$		
	$\max\lVert(R-\lambda_k I)x_k\rVert_2$	$\lVert X^T X - I\rVert_F$
Godunov Method	$5.5257061611023821e-14$	$8.7562001183895331e-13$
EISPACK Inverse Iteration	$1.7830382331966977e-13$	$3.7768280761380130e-12$
LAPACK Inverse Iteration	$2.3600706743928029e-16$	$1.3574708086966272e-14$
Godunov - Inverse Iteration	$2.3918916617431402e-16$	$9.4345051360760012e-15$

Table 5. Error estimates of the eigenvectors $X = |x_k|_{k=1,\ldots,n}$ of R, corresponding to eigenvalues $\tilde{\lambda}$ computed with maximum absolute deviation $\Delta = 4.4408920985006262e-16$ from the exact eigenvalues λ.

$\max\lvert\tilde{\lambda_k}(R) - \lambda_k(R)\rvert = 2.7755575615628914e-16,\ k = 1,\ldots,n$		
	$\max\lVert(R-\lambda_k I)x_k\rVert_2$	$\lVert X^T X - I\rVert_F$
Godunov Method	$4.6849824383640486e-14$	$6.0971993995822085e-13$
EISPACK Inverse Iteration	$1.9939253282522608e-13$	$1.4142135623730951e+00$
LAPACK Inverse Iteration	$1.3699144518926750e-16$	$1.4142135623730951e+00$
Godunov - Inverse Iteration	$1.3510126972303390e-16$	$1.4246653384402244e-14$

Table 6. Error estimates of the eigenvectors $X = |x_k|_{k=1,\ldots,n}$ of R, corresponding to eigenvalues $\tilde{\lambda}$ computed with maximum absolute deviation $\Delta = 2.7755575615628914e-16$ from the exact eigenvalues λ.

4. Conclusions

In this paper we presented a new robust procedure (algorithm 2) for computing eigenvectors of symmetric tridiagonal matrices. We use eigenvectors computed according to the Godunov's method as very accurate starting vectors in the Inverse Iteration. With starting eigenvectors nearly orthogonal, there is no need to apply Modified Gram-Schmidt orthogonalization, reducing the worst case complexity of the algorithm to $O(n^2)$ floating point operations. Godunov's method uses bisection algorithm to compute the smallest machine representable intervals that are guaranteed to contain eigenvalues of the tridiagonal matrix [2]. We use the right bounds of these eigenvalue intervals as the shifts in the Inverse Iteration in order to avoid the breakdown of the iteration, which may occur with more accurate shifts. In most experiments on the system without directed rounding (IEEE double precision, GNU C compiler, Pentium II processor) the new procedure converged in just one Inverse Iteration step, giving more accurate results than the Godunov's algorithm, and at least as accurate results as the standard Inverse Iteration procedures.

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