Diagonal pivoting methods for solving tridiagonal systems without interchanges

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Summary

Problem: Solve

$$Tx = b,$$

where T is unsymmetric, tridiagonal, and nonsingular.

Challenge:

- Some applications (e.g., bi-conjugate gradient) do not allow interchanges
- GEPP: stable but requires interchanges

Approach: Use LBM^T where L and M are lower triangular and B is block diagonal with 1×1 and 2×2 blocks. Can demonstrate backward stability.

Background

Symmetric tridiagonal:

- Bunch (1974)
- Bunch and Kaufman (1977)
- Bunch and RM (2005, 2006)
- Fang and O'Leary (2006)

Composite-step BiCG:

- Bank and Chan (1994)

Stability analysis:

- Higham (lots)

Notation

Let

$$T = \begin{bmatrix} \alpha_1 & \gamma_2 & 0 & \cdots & 0 \\ \beta_2 & \alpha_2 & \gamma_3 & \ddots & \vdots \\ 0 & \beta_3 & \alpha_3 & \ddots & 0 \\ \vdots & \ddots & \ddots & \ddots & \gamma_n \\ 0 & \cdots & 0 & \beta_n & \alpha_n \end{bmatrix}$$

and

$$\|T\|_{\max} = \max_{i,j} |T_{i,j}|.$$

Tridiagonal matrices

Partition

$$T = \begin{array}{c} \\ d \\ n-d \end{array} \begin{array}{c} \begin{array}{cc} d & n-d \end{array} \\ \left[\begin{array}{cc} B_1 & T_{12}^T \\ T_{21} & T_{22} \end{array} \right] \end{array}$$

T nonsingular $\Rightarrow B_1$ nonsingular for $d = 1$ or 2: Note that

$$B_1 = [\alpha_1] \quad \text{or} \quad \begin{bmatrix} \alpha_1 & \gamma_2 \\ \beta_2 & \alpha_2 \end{bmatrix}$$

Then

$$\alpha_1 = 0 \text{ and } \Delta = \alpha_1\alpha_2 - \beta_2\gamma_2 = 0 \implies \beta_2 = 0 \text{ or } \gamma_2 = 0$$
$$\implies T \text{ has a zero column or row}$$
$$\implies T \text{ is singular.}$$

Tridiagonal matrices

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$$T = \begin{array}{c} \\ d \\ n-d \end{array} \begin{array}{c} \begin{array}{cc} d & n-d \end{array} \\ \begin{bmatrix} B_1 & T_{12}^T \\ T_{21} & T_{22} \end{bmatrix} \end{array}$$

T nonsingular $\Rightarrow B_1$ nonsingular for $d = 1$ or 2. Thus

$$T = \begin{bmatrix} I_d & 0 \\ T_{21}B_1^{-1} & I_{n-d} \end{bmatrix} \begin{bmatrix} B_1 & 0 \\ 0 & T_{22} - T_{21}B_1^{-1}T_{12}^T \end{bmatrix} \begin{bmatrix} I_d & B_1^{-1}T_{12}^T \\ 0 & I_{n-d} \end{bmatrix}.$$

Tridiagonal matrices

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Schur complement $T_{22} - T_{21}B_1^{-1}T_{12}^T$ is tridiagonal:

$$T_{22} - \frac{\beta_2\gamma_2}{\alpha_1} e_1^{(n-1)} e_1^{(n-1)T} \qquad \text{or} \qquad T_{22} - \left(\frac{\alpha_1\beta_3\gamma_3}{\Delta} \right) e_1^{(n-2)} e_1^{(n-2)T}.$$

Tridiagonal matrices

Partition

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Compute recursively to obtain

$$T = LBM^T$$

where L and M are lower triangular and B is block diagonal with 1×1 and 2×2 blocks. **Question:** How to choose size of pivot d?

Proposed pivoting strategy

If $d = 1$, then

$$T = \left[\begin{array}{c|c} 1 & \\ \hline \beta_2/\alpha_1 & L_2 \end{array}\right] \left[\begin{array}{c|c} \alpha_1 & \\ \hline & B_2 \end{array}\right] \left[\begin{array}{c|c} 1 & \gamma_2/\alpha_1 \\ \hline & M_2^T \end{array}\right]$$

If $d = 2$, then

$$T = \left[\begin{array}{cc|c} 1 & & \\ & 1 & \\ \hline -\frac{\beta_2\beta_3}{\Delta} & \frac{\alpha_1\beta_3}{\Delta} & L_2 \end{array}\right] \left[\begin{array}{cc|c} \alpha_1 & \gamma_2 & \\ \beta_2 & \alpha_2 & \\ \hline & & B_2 \end{array}\right] \left[\begin{array}{cc|c} 1 & & -\frac{\gamma_2\gamma_3}{\Delta} \\ & 1 & \frac{\alpha_1\gamma_3}{\Delta} \\ \hline & & M_2^T \end{array}\right]$$

where $\Delta = \alpha_1\alpha_2 - \beta_2\gamma_2$.

Choose pivot size that yields smaller elements in L and M.

Proposed pivoting strategy

If $d = 1$, then

$$T = \left[\begin{array}{c|c} 1 & \\ \hline \beta_2/\alpha_1 & \\ & L_2 \end{array}\right] \left[\begin{array}{c|c} \alpha_1 & \\ \hline & \\ & B_2 \end{array}\right] \left[\begin{array}{c|c} 1 & \gamma_2/\alpha_1 \\ \hline & \\ & M_2^T \end{array}\right]$$

If $d = 2$, then

$$T = \left[\begin{array}{cc|c} 1 & & \\ & 1 & \\ \hline -\frac{\beta_2\beta_3}{\Delta} & \frac{\alpha_1\beta_3}{\Delta} & \\ & & L_2 \end{array}\right] \left[\begin{array}{cc|c} \alpha_1 & \gamma_2 & \\ \beta_2 & \alpha_2 & \\ \hline & & \\ & & B_2 \end{array}\right] \left[\begin{array}{cc|c} 1 & & -\frac{\gamma_2\gamma_3}{\Delta} \\ & 1 & \frac{\alpha_1\gamma_3}{\Delta} \\ \hline & & \\ & & M_2^T \end{array}\right]$$

where $\Delta = \alpha_1\alpha_2 - \beta_2\gamma_2$. **Criterion #1:** Choose a 1×1 pivot if

$$\max\left\{\frac{|\beta_2|}{|\alpha_1|}, \frac{|\gamma_2|}{|\alpha_1|}\right\} \leq \max\ \kappa \left\{\frac{|\beta_2\beta_3|}{|\Delta|}, \frac{|\alpha_1\beta_3|}{|\Delta|}, \frac{|\gamma_2\gamma_3|}{|\Delta|}, \frac{|\alpha_1\gamma_3|}{|\Delta|}\right\}.$$

Proposed pivoting strategy

Criterion #1: Equivalently, choose a 1×1 pivot if

$$|\Delta| \cdot \max\{|\beta_2|, |\gamma_2|\} \;\le\; |\alpha_1| \cdot \max\; \kappa\{|\beta_2\beta_3|, |\alpha_1\beta_3|, |\gamma_2\gamma_3|, |\alpha_1\gamma_3|\}$$

(**Intuition:** a 2×2 pivot is closer to being singular than a 1×1 pivot is to 0)

Criterion #2: Choose a 1×1 pivot if

$$|\alpha_1\alpha_2| \ge \kappa|\beta_2\gamma_2|.$$

(LBM^T reduces to the LDM^T factorization if T is positive definite).

Constant: $\kappa = (\sqrt{5} - 1)/2 \approx 0.62$ (Bunch (1974))

Proposed pivoting strategy

Algorithm 1.

$\kappa = (\sqrt{5} - 1)/2 \approx 0.62$

$\Delta = \alpha_1 \alpha_2 - \beta_2 \gamma_2$

if $|\Delta| \cdot \max\{|\beta_2|, |\gamma_2|\} \leq |\alpha_1| \cdot \max \kappa\{|\beta_2\beta_3|, |\alpha_1\beta_3|, |\gamma_2\gamma_3|, |\alpha_1\gamma_3|\}$

or $|\alpha_1\alpha_2| \geq \kappa|\beta_2\gamma_2|$

$d_I = 1$

else

$d_I = 2$

end

Alternative pivoting strategy

Algorithm 2.

$\kappa = (\sqrt{5}-1)/2 \approx 0.62$

$\sigma_1 = \max\{|\alpha_2|, |\gamma_2|, |\beta_2|, |\gamma_3|, |\beta_3|\}$

if $|\alpha_1|\sigma_1 \geq \kappa|\beta_2\gamma_2|$,

$d_{II} = 1$

else

$d_{II} = 2$

end

$$T = \begin{bmatrix} \alpha_1 & \gamma_2 & 0 & \cdots & 0 \\ \beta_2 & \alpha_2 & \gamma_3 & \ddots & \vdots \\ 0 & \beta_3 & \alpha_3 & \ddots & 0 \\ \vdots & \ddots & \ddots & \ddots & \gamma_n \\ 0 & \cdots & 0 & \beta_n & \alpha_n \end{bmatrix}$$

(cf. Bunch-Kaufman strategy for symmetric tridiagonal matrices – different from the more general Bunch-Kaufman LBL^T).

Pivoting strategies

Lemma. *If* $d_I = 1$*, then* $d_{II} = 1$*. If* $d_{II} = 2$*, then* $d_I = 2$*. And, if* $d_I = 2$ *and* $d_{II} = 1$*, then the subsequent pivot size* $\tilde{d}_{II}$ *is 1.*

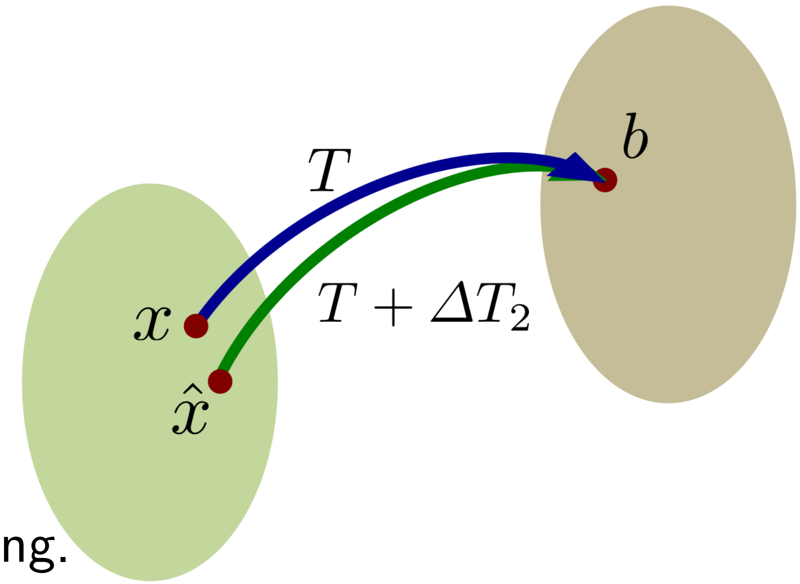
Summary: The two pivoting strategies differ only when the first strategy chooses a 2×2 pivot while the alternative chooses two 1×1 pivots.

Main theorem

Theorem. *Let $T \approx \hat{L}\hat{B}\hat{M}^T$ be the computed LBM^T factorization of the unsymmetric tridiagonal matrix $T \in \mathbb{R}^{n\times n}$ using Algorithm 1 or 2. Assume that all linear systems $Ey = f$ involving 2×2 pivots E are solved using the explicit inverse. Then*

$$T - \hat{L}\hat{B}\hat{M}^T = \Delta T_1, \quad \textit{and} \quad (T + \Delta T_2)\hat{x} = b,$$

where $\|\Delta T_i\|_{\max} \le cu\|T\|_{\max} + O(u^2)$, for $i = 1, 2$, where c is a constant.



Summary: $\hat{x}$ is the exact solution to a nearby problem.

Proof: Long and not particularly enlightening.

Numerical results

Obtained 16 unsymmetric tridiagonal matrices from Dhillon (1998) and Hargreaves (2004) on estimating condition numbers of tridiagonal matrices.

Matrix type	Description
1	Random elements (uniformly distributed on $[-1, 1]$).
2	Preassigned condition number with one very small singular value: `gallery('randsvd',n,1e15,2,1,1)`.
3	Preassigned condition number with geometric distribution of singular values: `gallery('randsvd',n,1e15,3,1,1)`.
7	Ill-conditioned, tridiagonal: `gallery('dorr',n,1e-4)`.
12	Toeplitz: main diagonal zero, each off-diagonal a random number (uniformly distributed on $[-1, 1]$).
15	Tridiagonal with main diagonal zero and known eigenvalues: `gallery('clement',n,0)`.

Numerical results

Generated 50×50 matrices of each type and computed $\|A\hat{x} - b\|_2$:

Matrix Type	Algorithm 1	Algorithm 2	GEPP	Cond. Num.
1	1.437796e-014	1.289799e-014	8.567857e-015	2.942402e+002
2	5.012055e-003	5.012055e-003	1.121297e-003	8.731214e+014
3	1.380824e-003	1.108818e-003	8.331566e-004	1.001503e+015
7	3.328680e+002	3.328680e+002	5.128745e+002	7.574961e+016
12	4.198353e-010	4.198353e-010	1.810847e-010	5.673349e+007
15	1.753491e-001	1.753491e-001	1.004420e-001	3.449791e+015

Conclusion: GEPP performs slightly better than LBM^T, but results are comparable.

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Future work: Extension to unsymmetric Lanczos / bi-conjugate gradient method.

References

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google: roummel

Thank you.