

Fast and accurate computations with Totally Nonnegative Quasiseparable Matrices

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- 1 Quasiseparable matrices
- 2 Goals of the talk
- 3 Neville elimination and quasiseparable matrices
- 4 Totally Nonnegative (TN) quasiseparable matrices
- 5 Solving quasiseparable linear systems
- 6 Error analysis for quasiseparable linear systems
- 7 Conclusions and future work

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Quasiseparable matrices (I): Definition

Definition

A square matrix C is **quasiseparable of order** (n_L, n_U) if

- every submatrix of C entirely located in the **strictly lower (resp. upper) triangular part** of C **have rank at most** n_L (resp. n_U), and
- at least one of these submatrices has rank equal to n_L (resp. n_U).

Remark

In this talk, we are interested only in the order $(1, 1)$ and for brevity the simple term **quasiseparable** is used instead of $(1, 1)$ -quasiseparable.

It is necessary and sufficient that the following submatrices have rank at most 1:

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Quasiseparable matrices (II)

$$C = \begin{bmatrix} \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times \end{bmatrix}$$

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Green's quasiseparable matrices (I)

Definition (Green's quasiseparable matrices)

A square matrix G is **Green's quasiseparable of order $(1, 1)$** if

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Parametrization of quasiseparable matrices

Theorem (Eidelman and Gohberg (1999))

The set of $n \times n$ quasiseparable matrices can be parameterized in terms of $7n - 8$ independent parameters or generators.

Example (Every 5×5 quasiseparable matrix is of the form)

$$C = \begin{bmatrix} \boxed{d_1} & g_1 h_2 & g_1 b_2 h_3 & g_1 b_2 b_3 h_4 & g_1 b_2 b_3 b_4 h_5 \\ p_2 q_1 & \boxed{d_2} & g_2 h_3 & g_2 b_3 h_4 & g_2 b_3 b_4 h_5 \\ p_3 a_2 q_1 & p_3 q_2 & \boxed{d_3} & g_3 h_4 & g_3 b_4 h_5 \\ p_4 a_3 a_2 q_1 & p_4 a_3 q_2 & p_4 q_3 & \boxed{d_4} & g_4 h_5 \\ p_5 a_4 a_3 a_2 q_1 & p_5 a_4 a_3 q_2 & p_5 a_4 q_3 & p_5 q_4 & \boxed{d_5} \end{bmatrix}$$

Remark

There are seven vectors (families) of parameters: $p_{2:n}$, $a_{2:n-1}$, $q_{1:n-1}$, $d_{1:n}$, $g_{1:n-1}$, $b_{2:n-1}$, $h_{2:n}$.

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Parametrization of Green's quasiseparable

Theorem

The set of $n \times n$ Green's quasiseparable matrices can be parameterized in terms of $6n - 2$ parameters with **the constraints** $p_i q_i = g_i h_i$ for $i = 1 : n$.

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Highlights on research on quasiseparable matrices (I)

- During the **last six years an intense research** has been performed on quasiseparable matrices.
- **Many researchers from different countries:** Belgium, Check Republic, Italy, Israel, Russia, USA...
- **Quasiseparable matrices appear in many applications:** systems theory and signal processing, discretization of integral equations, covariance matrices in multivariate statistics, discretization of elliptic PDEs....
- **Quasiseparable matrices include many important classes of matrices:** companion matrices of polynomials, **tridiagonal matrices and their inverses (Green's quasiseparable)**, unitary Hessenberg, banded matrices (for order larger than $(1, 1)$),.....
- Inverses of quasiseparable matrices are quasiseparable.

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Highlights on research on quasiseparable matrices (II)

- A main line of research has been the **development of structured fast algorithms by using the low number of parameters defining this class**. There are many algorithms and their costs are:

Problem	Cost of traditional algorithms	Cost of structured quasiseparable algs.
systems of equations	$O(n^3)$	$O(n)$
eigenvalues	$O(n^3)$	$O(n^2)$
singular values	$O(n^3)$	$O(n^2)$

- **The stability of these algorithms is not guaranteed and**, as far as we know, **error analysis have not been developed** even for the most simple cases.

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An historical TN-quasiseparable connection

In *Oscillation Matrices* (1941) by **Gantmacher and Krein** a **particular class of symmetric Green's quasiseparable** matrices is considered. These are called **single-pair** matrices and are defined as

$$S = \begin{bmatrix} p_1 q_1 & q_1 p_2 & q_1 p_3 & \dots \\ p_2 q_1 & p_2 q_2 & q_2 p_3 & \dots \\ p_3 q_1 & p_3 q_2 & p_3 q_3 & \dots \\ \vdots & \vdots & \vdots & \ddots \end{bmatrix} = \text{tril}(pq^T) + \text{strict-triu}(qp^T),$$

where all the numbers $p = [p_1, \dots, p_n]^T$, $q = [q_1, \dots, q_n]^T$ are nonzero.

These matrices are obtained from general Green's quasiseparable matrices by taking $a_i = b_i = 1$, $g_i = q_i$, and $h_i = p_i$.

Theorem (Gantmacher and Krein (1941))

S is **TN** if and only if all the numbers $p_1, \dots, p_n, q_1, \dots, q_n$ have the same sign and

$$\frac{q_1}{p_1} \leq \frac{q_2}{p_2} \leq \dots \leq \frac{q_n}{p_n}$$

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Goals of the talk

- We initiate the study of **stability of fast algorithms for quasiseparable matrices**, by presenting **rounding errors analysis** of the solution of **quasiseparable linear systems** by using a **bidiagonal factorization** followed by a **Björck-Pereyra** type algorithm.
- We prove that this algorithm is **componentwise backward stable in a strong sense**, i.e., preserving the structure, in the **TN-quasiseparable** case.
- For **Green's quasiseparable matrices** **simple forward errors bounds for this algorithm are presented** and we show that it is frequently **accurate**, independently of the traditional condition number of the matrix.
- We characterize **the set of nonsingular TN-quasiseparable** matrices through **the quasiseparable generators, the entries and the bidiagonal factorizations**. This extends Gantmacher and Krein's result.
- We briefly mention other results on accurate computations with **Green's quasiseparable matrices**.

Goals of the talk

- We initiate the study of **stability of fast algorithms for quasiseparable matrices**, by presenting **rounding errors analysis** of the solution of **quasiseparable linear systems** by using a **bidiagonal factorization** followed by a **Björck-Pereyra** type algorithm.
- We prove that this algorithm is **componentwise backward stable in a strong sense**, i.e., preserving the structure, in the **TN-quasiseparable** case.
- For **Green's quasiseparable matrices** **simple forward errors bounds for this algorithm are presented** and we show that it is frequently **accurate**, independently of the traditional condition number of the matrix.
- We characterize **the set of nonsingular TN-quasiseparable** matrices through **the quasiseparable generators, the entries and the bidiagonal factorizations**. This extends Gantmacher and Krein's result.
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- We develop error analysis and Gemignani does not.
- Gemignani deals with general (n_L, n_U) -order quasiseparable matrix and we only with $(1, 1)$ -order.
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- 2 Goals of the talk
- 3 Neville elimination and quasiseparable matrices**
- 4 Totally Nonnegative (TN) quasiseparable matrices
- 5 Solving quasiseparable linear systems
- 6 Error analysis for quasiseparable linear systems
- 7 Conclusions and future work

Brief summary on Neville elimination (I)

- It is a classic **procedure to create zeros in a matrix by adding to a row (resp. column) a multiple of the previous row (resp. column).**
- It is valid for any matrix, it is different than Gaussian elimination and it has different backward errors.
- **Without interchanges**, it was carefully analyzed by **Gasca and Peña** in a series of seminal papers in the 90s. In particular, its **matricial description** in terms of **bidiagonal factorizations** and its fundamental relationship with **total nonnegativity** were established.

Theorem (Gasca and Peña (1994))

A nonsingular matrix A is TN if and only if complete Neville elimination can be performed on A without row or column exchanges, with nonnegative multipliers and positive diagonal pivots.

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Brief summary on Neville elimination (II)

- **Neville elimination without exchanges adapts very well to the quasiseparable structure** (Gemignani 2008).
- The quasiseparable structure is destroyed by row or column exchanges.
- In this talk, **Neville elimination is never applied numerically**. It is a theoretical way to get formulae, in terms of the generators, for the **bidiagonal factors of the matrix**. These formulae are then used
 - 1 to develop fast algorithms,
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Bidiagonal factorizations (II)

Example (Bidiagonal factorization of a 5×5 matrix)

$$A = L^{(1)}L^{(2)}L^{(3)}L^{(4)}\mathbf{D}U^{(4)}U^{(3)}U^{(2)}U^{(1)},$$

$$\mathbf{D} = \begin{bmatrix} \times & & & & \\ & \times & & & \\ & & \times & & \\ & & & \times & \\ & & & & \times \end{bmatrix}$$

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Simplifying assumptions

- The generators of a quasiseparable matrix **are not unique**.
- We will assume (not essential) that for any C quasiseparable matrix

$$C(i, 1 : i - 1) = 0 \implies p_i = 0 \quad \text{and} \quad C(1 : i - 1, i) = 0 \implies h_i = 0$$

Example (5×5 quasiseparable matrix)

$$C = \begin{bmatrix} \boxed{d_1} & g_1 h_2 & g_1 b_2 h_3 & g_1 b_2 b_3 h_4 & g_1 b_2 b_3 b_4 h_5 \\ p_2 q_1 & \boxed{d_2} & g_2 h_3 & g_2 b_3 h_4 & g_2 b_3 b_4 h_5 \\ p_3 a_2 q_1 & p_3 q_2 & \boxed{d_3} & g_3 h_4 & g_3 b_4 h_5 \\ \hline p_4 a_3 a_2 q_1 & p_4 a_3 q_2 & p_4 q_3 & \boxed{d_4} & g_4 h_5 \\ \hline p_5 a_4 a_3 a_2 q_1 & p_5 a_4 a_3 q_2 & p_5 a_4 q_3 & p_5 q_4 & \boxed{d_5} \end{bmatrix}$$

$$C(4, 1 : 3) = [p_4 a_3 a_2 q_1 \quad p_4 a_3 q_2 \quad p_4 q_3] = 0 \implies p_4 = 0$$

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$$C(1 : 3, 4) = [g_1 b_2 b_3 h_4 \quad g_2 b_3 h_4 \quad g_3 h_4]^T = 0 \implies h_4 = 0$$

Similar for **Green's quasiseparable** matrices.

$$\ell_5 := \begin{cases} \frac{p_5 a_4}{p_4} \left(= \frac{g_{51}}{g_{41}} \right) & \text{if } p_4 \neq 0 \\ 0 & \text{if } p_4 = 0 \end{cases} \rightarrow E_5(-\ell_5) = \begin{bmatrix} 1 & & & & \\ & 1 & & & \\ & & 1 & & \\ & & & 1 & \\ & & & & -\ell_5 & 1 \end{bmatrix}$$

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rank one matrix $\Rightarrow \frac{g_{51}}{g_{41}} = \frac{g_{52}}{g_{42}} = \frac{g_{53}}{g_{43}} = \frac{g_{54}}{g_{44}}$

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$$p_5 q_5 = g_5 h_5 \implies g'_5 = g_5 - \ell_5 g_4 b_4$$

Bidiagonal factorization of Green's quasiseparable

Theorem

Complete Neville elimination runs without exchanges on a nonsingular $n \times n$ Green's quasiseparable matrix G specified by its generators if and only if

$$G = E_n(\ell_n) \cdots E_3(\ell_3) E_2(\ell_2) D E_2(u_2)^T E_3(u_3)^T \cdots E_n(u_n)^T,$$

where $D = \text{diag}(\mathbf{d}_1, \dots, \mathbf{d}_n)$, and

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$$\mathbf{d}_1 = p_1 q_1, \quad \mathbf{d}_i = p_i q_i - \ell_i u_i p_{i-1} q_{i-1} \quad \text{for } i = 2 : n$$

Remarks

- The **bidiagonal factorization of G is sparse: $3n - 2$ nontrivial entries**
- The bidiagonal factorization of G **can be computed through explicit formulae from generators** (also from entries) **in $O(n)$ flops.**

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Bidiagonal factorization of a quasiseparable matrix (I)

Theorem

Complete Neville elimination runs without exchanges on a nonsingular $n \times n$ quasiseparable matrix C specified by its generators if and only if

$$C = E_n(\ell_n) \cdots E_4(\ell_4) E_3(\ell_3) T E_3(u_3)^T E_4(u_4)^T \cdots E_n(u_n)^T,$$

where

$$\ell_i := \begin{cases} \frac{p_i a_{i-1}}{p_{i-1}} & \text{if } p_{i-1} \neq 0 \\ 0 & \text{if } p_{i-1} = 0 \end{cases} \quad u_i := \begin{cases} \frac{h_i b_{i-1}}{h_{i-1}} & \text{if } h_{i-1} \neq 0 \\ 0 & \text{if } h_{i-1} = 0 \end{cases}$$

and

$$T = \begin{bmatrix} y_1 & z_2 & & & & \\ x_2 & y_2 & z_3 & & & \\ & \ddots & \ddots & \ddots & & \\ & & & x_{n-1} & y_{n-1} & z_n \\ & & & & x_n & y_n \end{bmatrix},$$

has LDU factorization, where

Bidiagonal factorization of a quasiseparable matrix (II)

Theorem (continued)

$$x_2 = p_2 q_1, \quad x_j = p_j q_{j-1} - \ell_j d_{j-1} \quad \text{for } j = 3 : n$$

$$y_1 = d_1, \quad y_2 = d_2, \quad y_j = d_j - \ell_j g_{j-1} h_j - u_j p_j q_{j-1} + u_j \ell_j d_{j-1} \quad \text{for } j = 3 : n$$

$$z_2 = g_1 h_2, \quad z_j = g_{j-1} h_j - u_j d_{j-1} \quad \text{for } j = 3 : n$$

Remarks

- **We can compute through formulae from the generators** (or entries)

$$C = E_n(\ell_n) \cdots E_4(\ell_4) E_3(\ell_3) T E_3(u_3)^T E_4(u_4)^T \cdots E_n(u_n)^T,$$

- but, **to get the bidiagonal factorization**, it remains to compute with **usual Gaussian (Neville) elimination on a tridiagonal** matrix,

$$T = L^{(n-1)} D U^{(n-1)}.$$

- Total cost is $O(n)$ **flops** and the **bidiagonal factorization of C is sparse: $5n - 6$ nontrivial entries**

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TN quasiseparable and bidiagonal factorizations

Theorem

An $n \times n$ nonsingular matrix C is TN and quasiseparable **if and only if**

$$C = E_n(\ell_n) \cdots E_3(\ell_3) L^{(n-1)} D U^{(n-1)} E_3(u_3)^T \cdots E_n(u_n)^T,$$

with all the bidiagonal factors nonnegative and the diagonal entries of D positive.

Theorem

An $n \times n$ nonsingular matrix G is TN and Green's quasiseparable **if and only if**

$$G = E_n(\ell_n) \cdots E_2(\ell_2) D E_2(u_2)^T \cdots E_n(u_n)^T,$$

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with **all the bidiagonal factors nonnegative and the diagonal entries of D positive.**

Theorem (characterization in terms of the parameters)

Let G be an $n \times n$ Green's quasiseparable matrix specified by its generators. Then

$$G \text{ is nonsingular and TN} \iff \begin{cases} p_1 q_1 > 0, & \text{and} \\ p_i q_i - \left(\frac{p_i a_{i-1}}{p_{i-1}} \right) \left(\frac{h_i b_{i-1}}{h_{i-1}} \right) p_{i-1} q_{i-1} > 0, \\ \frac{p_i a_{i-1}}{p_{i-1}} \geq 0, \quad \frac{h_i b_{i-1}}{h_{i-1}} \geq 0, & \text{for } 2 \leq i \leq n \end{cases}$$

These conditions can be checked in $O(n)$ flops.

Theorem (characterization in terms of the entries)

Let G be an $n \times n$ Green's quasiseparable matrix. Then

$$G \text{ is nonsingular and TN} \iff \begin{cases} g_{ii} > 0, & 1 \leq i \leq n \\ g_{i,i-1} \geq 0, \quad g_{i-1,i} \geq 0, & 2 \leq i \leq n \\ \det G(i-1:i, i-1:i) > 0, & 2 \leq i \leq n \end{cases}$$

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$$T = \begin{bmatrix} y_1 & z_2 & & & & \\ x_2 & y_2 & z_3 & & & \\ & \ddots & \ddots & \ddots & & \\ & & x_{n-1} & y_{n-1} & z_n & \\ & & & x_n & y_n & \end{bmatrix},$$

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Theorem (continued)

Then, C is nonsingular and TN if and only if

- $l_i \geq 0$ and $u_i \geq 0$ for $i = 3 : n$.
- The tridiagonal matrix T is nonsingular and TN.
- If $p_j q_{j-1} = 0$, for some j , then $C(j : n, 1 : j - 1) = 0$.
- If $g_{j-1} h_j = 0$, for some j , then $C(1 : j - 1, j : n) = 0$.

These conditions can be checked in $O(n)$ flops.

$$C = \begin{bmatrix} \boxed{d_1} & g_1 h_2 & g_1 b_2 h_3 & g_1 b_2 b_3 h_4 & g_1 b_2 b_3 b_4 h_5 \\ p_2 q_1 & \boxed{d_2} & g_2 h_3 & g_2 b_3 h_4 & g_2 b_3 b_4 h_5 \\ p_3 a_2 q_1 & p_3 q_2 & \boxed{d_3} & g_3 h_4 & g_3 b_4 h_5 \\ p_4 a_3 a_2 q_1 & p_4 a_3 q_2 & p_4 q_3 = 0 & \boxed{d_4} & g_4 h_5 \\ p_5 a_4 a_3 a_2 q_1 & p_5 a_4 a_3 q_2 & p_5 a_4 q_3 & p_5 q_4 & \boxed{d_5} \end{bmatrix}$$

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Given a bidiagonal factorization...

Assume that for a **general matrix** A :

- We know a bidiagonal factorization

$$A = L^{(1)}L^{(2)} \dots L^{(n-1)}DU^{(n-1)} \dots U^{(2)}U^{(1)}.$$

- We want to solve $Ax = b$.

Then

$$L^{(1)}x^{(1)} = b, \quad L^{(2)}x^{(2)} = x^{(1)}, \quad \dots \quad L^{(n-1)}x^{(n-1)} = x^{(n-2)},$$

$$Dx^{(n)} = x^{(n-1)},$$

$$U^{(n-1)}x^{(n+1)} = x^{(n)}, \quad U^{(n-2)}x^{(n+2)} = x^{(n+1)}, \quad \dots \quad U^{(1)}x = x^{(2n-2)}$$

Observe that for quasiseparable matrices many of the bidiagonal systems are very simple and can be solved in two flops:

$$E_i(\alpha)z = y \iff z = E_i(-\alpha)y.$$

In fact, **all are of this type for Green's quasiseparable matrices.**

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The complete $O(n)$ quasiseparable algorithm

ALGORITHM 1

INPUT: **Generators** of C (resp. G) $n \times n$ quasiseparable (resp. Green's quasiseparable) matrix and vector b

OUTPUT: Solution of $Cx = b$ (resp. $Gx = b$)

- **Compute bidiagonal factorization with formulae** as in the first part of the talk:

$$C = E_n(\ell_n) \cdots E_3(\ell_3) L^{(n-1)} D U^{(n-1)} E_3(u_3)^T \cdots E_n(u_n)^T,$$

$$\text{(resp. } G = E_n(\ell_n) \cdots E_2(\ell_2) D E_2(u_2)^T \cdots E_n(u_n)^T \text{)}$$

- **Solve a sequence of bidiagonal systems** to get x as in the previous slide.

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Theorem

If Algorithm 1 is applied to solve $Cx = b$, where C is $n \times n$ **quasiseparable matrix**, and

$$E_n(\widehat{\ell}_n), \dots, E_3(\widehat{\ell}_3), \widehat{L}^{(n-1)}, \widehat{D}, \widehat{U}^{(n-1)}, E_3(\widehat{u}_3)^T, \dots, E_n(\widehat{u}_n)^T,$$

are the **computed bidiagonal factors of C** with *unit roundoff* ϵ , then **the computed solution \widehat{x} satisfies**

$$(C + E)\widehat{x} = b,$$

where

- **$(C + E)$ is quasiseparable**, and



$$|E| \leq \frac{27n\epsilon}{1 - 27n\epsilon} E_n(|\widehat{\ell}_n|) \cdots E_3(|\widehat{\ell}_3|) |\widehat{L}^{(n-1)}| |\widehat{D}| |\widehat{U}^{(n-1)}| E_3(|\widehat{u}_3|)^T \cdots E_n(|\widehat{u}_n|)^T$$

Comments on this backward error analysis

- Similar result for **Green's quasiseparable matrices**, preserving the Green's structure.
- It is very **tricky**.
- It requires a **delicate way to evaluate the formulae** for the bidiagonal/tridiagonal factors
- It combines
 - 1 **mixed backward-forward errors in terms of parameters and bidiagonal factors**, with
 - 2 **backward errors in terms of entries**.
- The **bound may be not satisfactory** if

$$E_n(|\hat{\ell}_n|) \cdots E_3(|\hat{\ell}_3|) |\hat{L}^{(n-1)}| |\hat{D}| |\hat{U}^{(n-1)}| E_3(|\hat{u}_3|)^T \cdots E_n(|\hat{u}_n|)^T \gg |C|$$

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Theorem

If Algorithm 1 is applied to solve $Cx = b$, where C is $n \times n$ **quasiseparable matrix**, and all the **computed bidiagonal factors of C are nonnegative** ($\text{diag } \hat{D} > 0$), then **the computed solution \hat{x} satisfies**

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Theorem

Let G be an $n \times n$ Green's quasiseparable matrix and define

$$\kappa_{GQ}(G) = \max_{2 \leq i \leq n} \frac{|g_{i,i} g_{i-1,i-1}| + |g_{i,i-1} g_{i-1,i}|}{|g_{i,i} g_{i-1,i-1} - g_{i,i-1} g_{i-1,i}|}.$$

Assume that Algorithm 1 is applied to solve $Gx = b$ with unit roundoff ϵ and that the **computed bidiagonal factors of G are nonnegative** (\hat{D} nonsingular). If

$$\frac{9\epsilon}{1 - 9\epsilon} \kappa_{GQ}(G) < \frac{1}{2},$$

then

- G is nonsingular and TN.
- The computed solution \hat{x} satisfies

$$|x - \hat{x}| \leq 2 \left(\frac{8n\epsilon}{1 - 8n\epsilon} + \kappa_{GQ}(G) \frac{9\epsilon}{1 - 9\epsilon} \right) \|G^{-1}\| \|b\|$$

Forward errors for TN-Green's quasiseparable (II)

$$|x - \hat{x}| \leq 2 \left(\frac{8n\epsilon}{1 - 8n\epsilon} + \kappa_{\mathbf{GQ}}(\mathbf{G}) \frac{9\epsilon}{1 - 9\epsilon} \right) \|G^{-1}\| \|b\|$$

- If $\epsilon \kappa_{\mathbf{GQ}}(\mathbf{G}) \ll 1$, this is a very satisfactory bound, because
- $\frac{\| |G^{-1}| \|b\| \|_{\infty}}{\|x\|_{\infty}} = \frac{\| |G^{-1}| \|b\| \|_{\infty}}{\|G^{-1}b\|_{\infty}}$ is moderate except for particular b 's.

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is a **condition number for this problem**.

- Note that

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- We know how to **compute in $O(n^2)$ flops eigenvalues and singular values of TN-Green's quasiseparable matrices with relative errors**

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- We have shown perfect componentwise backward stability in **solving linear systems through bidiagonalization** for **diagonally dominant** Green's quasiseparable matrices.

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Outline

- 1 Quasiseparable matrices
- 2 Goals of the talk
- 3 Neville elimination and quasiseparable matrices
- 4 Totally Nonnegative (TN) quasiseparable matrices
- 5 Solving quasiseparable linear systems
- 6 Error analysis for quasiseparable linear systems
- 7 Conclusions and future work**

Conclusions and future work

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- **It is fast and backward stable on TN-quasiseparable.**
- Simple **forward error bounds for TN Green's quasiseparable** available.
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