



CSCI 5304

Fall 2021

#### COMPUTATIONAL ASPECTS OF MATRIX THEORY

 $egin{array}{lll} {\it Class\ time} & : & MW\ 4:00-5:15\ pm \\ {\it Room} & : & {\it Keller\ 3-230\ or\ Online} \\ {\it Instructor} & : & {\it Daniel\ Boley} \\ \end{array}$ 

Lecture notes:

http://www-users.cselabs.umn.edu/classes/Fall-2021/csci5304/

August 27, 2021

#### **SOLVING LINEAR SYSTEMS OF EQUATIONS**

- Background on linear systems
- Gaussian elimination and the Gauss-Jordan algorithms
- The LU factorization
- Gaussian Elimination with pivoting permutation matrices.
- Case of banded systems

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### Background: Linear systems

**The Problem:** A is an  $n \times n$  matrix, and b a vector of  $\mathbb{R}^n$ . Find x such that:

$$Ax = b$$

ightharpoonup x is the unknown vector, b the right-hand side, and A is the coefficient matrix

## Example:

$$\begin{cases} 2x_1 + 4x_2 + 4x_3 = 6 \\ x_1 + 5x_2 + 6x_3 = 4 \text{ or } \begin{pmatrix} 2 & 4 & 4 \\ 1 & 5 & 6 \\ x_1 + 3x_2 + & x_3 = 8 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 6 \\ 4 \\ 8 \end{pmatrix}$$

**∠** Solution of above system ?

> Standard mathematical solution by Cramer's rule:

$$x_i = \det(A_i)/\det(A)$$

 $A_i = \text{matrix obtained by replacing } i\text{-th column by } b.$ 

Note: This formula is useless in practice beyond n=3 or n=4.

#### Three situations:

- 1. The matrix  ${m A}$  is nonsingular. There is a unique solution given by  ${m x} = {m A}^{-1}{m b}$ .
- 2. The matrix A is singular and  $b \in \text{Ran}(A)$ . There are infinitely many solutions.
- 3. The matrix A is singular and  $b \notin \operatorname{Ran}(A)$ . There are no solutions.

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GvL 3.{1,3,5} – Systems

**Example:** (1) Let  $A=\begin{pmatrix} 2 & 0 \\ 0 & 4 \end{pmatrix}$   $b=\begin{pmatrix} 1 \\ 8 \end{pmatrix}$  . A is nonsingular  $\blacktriangleright$  a unique solution  $x=\begin{pmatrix} 0.5 \\ 2 \end{pmatrix}$  .

**Example:** (2) Case where A is singular &  $b \in \operatorname{Ran}(A)$ :

$$A=egin{pmatrix} 2 & 0 \ 0 & 0 \end{pmatrix}, \quad b=egin{pmatrix} 1 \ 0 \end{pmatrix}.$$

- lacksquare infinitely many solutions:  $x(lpha)=egin{pmatrix} 0.5 \ lpha \end{pmatrix} \ \ orall \ lpha.$
- **Example:** (3) Let A same as above, but  $b = \begin{pmatrix} 1 \\ 1 \end{pmatrix}$ .
- No solutions since 2nd equation cannot be satisfied

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## Triangular linear systems

## Example:

$$egin{pmatrix} 2 & 4 & 4 \ 0 & 5 & -2 \ 0 & 0 & 2 \end{pmatrix} egin{pmatrix} x_1 \ x_2 \ x_3 \end{pmatrix} = egin{pmatrix} 2 \ 1 \ 4 \end{pmatrix}$$

- $\triangleright$  One equation can be trivially solved: the last one.  $x_3 = 2$
- $ightharpoonup x_3$  is known we can now solve the 2nd equation:

$$5x_2 - 2x_3 = 1 \rightarrow 5x_2 - 2 \times 2 = 1 \rightarrow x_2 = 1$$

 $\triangleright$  Finally  $x_1$  can be determined similarly:

$$2x_1 + 4x_2 + 4x_3 = 2 \rightarrow \dots \rightarrow x_1 = -5$$

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#### ALGORITHM: 1. Back-Substitution algorithm

For 
$$i=n:-1:1$$
 do:  $t:=b_i$  For  $j=i+1:n$  do  $t:=t-a_{ij}x_j$   $t:=b_i-(a_{i,i+1:n},x_{i+1:n})$   $t:=b_i-a_i$  inner product  $x_i=t/a_{ii}$ 

- $\blacktriangleright$  We must require that each  $a_{ii} \neq 0$
- Operation count?

## Column version of back-substitution

Back-Substitution algorithm. Column version

For 
$$j=n:-1:1$$
 do:  $x_j=b_j/a_{jj}$  For  $i=1:j-1$  do  $b_i:=b_i-x_j*a_{ij}$  End

Justify the above algorithm [Show that it does indeed compute the solution]

Analogous algorithms for lower triangular systems.

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## Linear Systems of Equations: Gaussian Elimination

Back to arbitrary linear systems.

<u>Principle of the method:</u> Since triangular systems are easy to solve, we will transform a linear system into one that is triangular. Main operation: combine rows so that zeros appear in the required locations to make the system triangular.

Notation: use a Tableau:

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# Linear Systems of Equations: Gaussian Elimination

Go back to original system. Step 1 must transform:

$$egin{bmatrix} 2 & 4 & 4 & 2 \ 1 & 3 & 1 & 1 \ 1 & 5 & 6 & -6 \ \end{bmatrix}$$
 into:  $egin{bmatrix} x & x & x & x \ 0 & x & x & x \ 0 & x & x & x \ \end{bmatrix}$ 

 $row_2 := row_2 - \frac{1}{2} \times row_1$ :  $row_3 := row_3 - \frac{1}{2} \times row_1$ :

$$egin{bmatrix} 2 & 4 & 4 & 2 \ 0 & 1 & -1 & 0 \ 0 & 3 & 4 & -7 \ \end{bmatrix}$$

Main operation used: scaling and adding rows.

**Example:** Replace row2 by: row2 -  $\frac{1}{2}$ \*row1:

➤ This is equivalent to:

$$\begin{bmatrix} 1 & 0 & 0 \\ -\frac{1}{2} & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \times \begin{bmatrix} 2 & 4 & 4 & 2 \\ 1 & 3 & 1 & 1 \\ 1 & 5 & 6 & -6 \end{bmatrix} = \begin{bmatrix} 2 & 4 & 4 & 2 \\ 0 & 1 & -1 & 0 \\ 1 & 5 & 6 & -6 \end{bmatrix}$$

➤ The left-hand matrix is of the form

$$M = I - ve_1^T$$
 with  $v = egin{pmatrix} 0 \ rac{1}{2} \ 0 \end{pmatrix}$ 

GvL 3.{1,3,5} – Systems

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> Equivalent to

$$\begin{vmatrix} 1 & 0 & 0 \\ -\frac{1}{2} & 1 & 0 \\ -\frac{1}{2} & 0 & 1 \end{vmatrix} \times \begin{vmatrix} 2 & 4 & 4 & 2 \\ 1 & 3 & 1 & 1 \\ 1 & 5 & 6 & -6 \end{vmatrix} = \begin{vmatrix} 2 & 4 & 4 & 2 \\ 0 & 1 & -1 & 0 \\ 0 & 3 & 4 & -7 \end{vmatrix}$$

$$[A,b] 
ightarrow [M_1A,M_1b]; \;\; M_1 = I - v^{(1)} e_1^T; \;\; v^{(1)} = egin{pmatrix} 0 \ rac{1}{2} \ rac{1}{2} \end{pmatrix}$$

New system  $A_1x = b_1$ . Step 2 must now transform:

$$row_3 := row_3 - 3 imes row_2 : 
ightarrow egin{bmatrix} 2 & 4 & 4 & 2 \ 0 & 1 & -1 & 0 \ 0 & 0 & 7 & -7 \ \end{pmatrix}$$

Equivalent to

$$\begin{vmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & -3 & 1 \end{vmatrix} \times \begin{vmatrix} 2 & 4 & 4 & 2 \\ 0 & 1 & -1 & 0 \\ 0 & 3 & 4 & -7 \end{vmatrix} = \begin{vmatrix} 2 & 4 & 4 & 2 \\ 0 & 1 & -1 & 0 \\ 0 & 0 & 7 & -7 \end{vmatrix}$$

Second transformation is as follows:

$$[A_1,b_1] 
ightarrow [M_2A_1,M_2b_1]; \; M_2 = I - v^{(2)}e_2^T; \; v^{(2)} = egin{pmatrix} 0 \ 0 \ 3 \end{pmatrix}$$

➤ Triangular system ➤ Solve.

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Row k

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## ALGORITHM: 2. Gaussian Elimination

- 1. For k = 1 : n 1 Do:
- 2. For i = k + 1 : n Do:
- 3.  $piv := a_{ik}/a_{kk}$
- 4. For j := k + 1 : n + 1 Do :
- $5. a_{ij} := a_{ij} piv * a_{kj}$
- 6. End
- 6. End
- 7. End
- Operation count:

$$T = \sum_{k=1}^{n-1} \sum_{i=k+1}^{n} [1 + \sum_{j=k+1}^{n+1} 2] = \sum_{k=1}^{n-1} \sum_{i=k+1}^{n} (2(n-k) + 3) = ...$$

Complete the above calculation. Order of the cost?

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#### The LU factorization

Now ignore the right-hand side from the transformations.

Observation: Gaussian elimination is equivalent to n-1 successive Gaussian transformations, i.e., multiplications with matrices of the form  $M_k=I-v^{(k)}e_k^T$ , where the first k components of  $v^{(k)}$  equal zero.

ightharpoonup Set  $A_0 \equiv A$ 

$$A o M_1 A_0 = A_1 o M_2 A_1 = A_2 o M_3 A_2 = A_3 \cdots \ o M_{n-1} A_{n-2} = A_{n-1} \equiv U$$

ightharpoonup Last  $A_k \equiv U$  is an upper triangular matrix.

GvL 3.{1,3,5} — Systems

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ightharpoonup At each step we have:  $A_k = M_{k+1}^{-1} A_{k+1}$  . Therefore:

$$A_0 = M_1^{-1} A_1$$

$$= M_1^{-1} M_2^{-1} A_2$$

$$= M_1^{-1} M_2^{-1} M_3^{-1} A_3$$

$$= \dots$$

$$= M_1^{-1} M_2^{-1} M_3^{-1} \cdots M_{n-1}^{-1} A_{n-1}$$

- $L = M_1^{-1} M_2^{-1} M_3^{-1} \cdots M_{n-1}^{-1}$
- ightharpoonup Note: L is Lower triangular,  $A_{n-1}$  is upper triangular
- lacksquare LU decomposition : A=LU

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A matrix  $oldsymbol{A}$  has an LU decomposition if

$$\det(A(1:k,1:k)) \neq 0$$
 for  $k = 1, \dots, n-1$ .

In this case, the determinant of  $\boldsymbol{A}$  satisfies:

$$\det A = \det(U) = \prod_{i=1}^n u_{ii}$$

If, in addition,  $\boldsymbol{A}$  is nonsingular, then the LU factorization is unique.

## How to get L?

$$L = M_1^{-1} M_2^{-1} M_3^{-1} \cdots M_{n-1}^{-1}$$

- Consider only the first 2 matrices in this product.
- ightharpoonup Note  $M_k^{-1}=(I-v^{(k)}e_k^T)^{-1}=(I+v^{(k)}e_k^T).$  So:

$$M_1^{-1}M_2^{-1} = (I + v^{(1)}e_1^T)(I + v^{(2)}e_2^T) = I + v^{(1)}e_1^T + v^{(2)}e_2^T.$$

➤ Generally,

$$M_1^{-1}M_2^{-1}\cdots M_k^{-1} = I + v^{(1)}e_1^T + v^{(2)}e_2^T + \cdots v^{(k)}e_k^T$$

The L factor is a lower triangular matrix with ones on the diagonal. Column k of L, contains the multipliers  $l_{ik}$  used in the k-th step of Gaussian elimination.

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Practical use: Show how to use the LU factorization to solve linear systems with the same matrix A and different b's.

LU factorization of the matrix  $A = \begin{pmatrix} 2 & 4 & 4 \\ 1 & 5 & 6 \\ 1 & 3 & 1 \end{pmatrix}$ ?

True or false: "Computing the LU factorization of matrix A involves more arithmetic operations than solving a linear system Ax = b by Gaussian elimination".

#### Gauss-Jordan Elimination

Principle of the method: We will now transform the system into one that is even easier to solve than triangular systems, namely a diagonal system. The method is very similar to Gaussian Elimination. It is just a bit more expensive.

Back to original system. Step 1 must transform:

2	4	4	2		$\boldsymbol{x}$	$\boldsymbol{x}$	$\boldsymbol{x}$	$\boldsymbol{x}$
1	3	1	1	into:	0	$\boldsymbol{x}$	$\boldsymbol{x}$	$ oldsymbol{x}$
1	<b>5</b>	6	<b>-6</b>		0	$\boldsymbol{x}$	$\boldsymbol{x}$	$ oldsymbol{x} $

GvL 3.{1,3,5} - Systems

#### There is now a third step:

 $row_1 := row_1 - \frac{8}{7} \times row_3$ :  $row_2 := row_2 - \frac{-1}{7} \times row_3$ :

$$egin{bmatrix} 2 & 0 & 0 & 10 \ 0 & 1 & -1 & 0 \ 0 & 0 & 7 & -7 \ \end{bmatrix}$$

$$\begin{array}{ccc|c} 2 & 0 & 0 & 10 \\ 0 & 1 & 0 & 1 \\ 0 & 0 & 7 & -7 \end{array}$$

Solution:  $x_3 = -1$ ;  $x_2 = -1$ ;  $x_1 = 5$ 

 $row_2 := row_2 - 0.5 \times row_1$ :  $row_3 := row_3 - 0.5 \times row_1$ :

$$\begin{bmatrix} 2 & 4 & 4 & 2 \\ 0 & 1 & -1 & 0 \\ 0 & 3 & 4 & -7 \end{bmatrix}$$

Step 2: 0

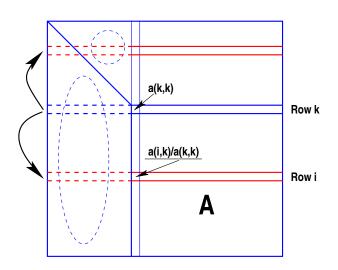
 $1 \quad -1 \quad 0 \quad | \text{ into: } \quad 0 \quad x \quad x \mid x$  $\boldsymbol{x} | \boldsymbol{x}$ 

 $row_1 := row_1 - 4 \times row_2$ :  $row_3 := row_3 - 3 \times row_2$ :

$$\begin{bmatrix} 2 & 0 & 8 & 2 \\ 0 & 1 & -1 & 0 \\ 0 & 3 & 4 & -7 \end{bmatrix}$$

GvL 3.{1,3,5} - Systems

GvL 3.{1,3,5} - Systems



#### ALGORITHM: 3. Gauss-Jordan elimination

- 1. For k = 1 : n Do:
- 2. For i = 1 : n and if i! = k Do :
- $3. piv := a_{ik}/a_{kk}$
- 4. For j := k + 1 : n + 1 Do :
- $5. a_{ij} := a_{ij} piv * a_{kj}$
- 6. End
- 6. End
- 7. End

#### ➤ Operation count:

$$T = \sum_{k=1}^{n} \sum_{i=1}^{n-1} [1 + \sum_{j=k+1}^{n+1} 2] = \sum_{k=1}^{n} \sum_{i=1}^{n-1} (2(n-k) + 3) = \cdots$$

Complete the above calculation. Order of the cost? How does it compare with Gaussian Elimination?

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### Gaussian Elimination: Partial Pivoting

Consider again Gaussian Elimination for the linear system

$$\left\{ \begin{array}{lll} 2x_1 + 2x_2 + 4x_3 = & 2 \\ x_1 + & x_2 + & x_3 = & 1 & \mathrm{Or:} \end{array} \right. \left. \begin{array}{lll} 2 & 2 & 4 & 2 \\ 1 & 1 & 1 & 1 \\ 1 & 4 & 6 & -5 \end{array} \right.$$

 $row_2 := row_2 - \frac{1}{2} \times row_1$ :  $row_3 := row_3 - \frac{1}{2} \times row_1$ :

$$egin{bmatrix} 2 & 2 & 4 & 2 \ 0 & 0 & -1 & 0 \ 1 & 4 & 6 & -5 \ \end{bmatrix}$$

$$\begin{bmatrix} 2 & 2 & 4 & 2 \\ 0 & 0 & -1 & 0 \\ 0 & 3 & 4 & -6 \end{bmatrix}$$

Pivot  $a_{22}$  is zero. Solution : permute rows 2 and 3:

GvL 3.{1,3,5} - Systems

### Gaussian Elimination with Partial Pivoting

## Partial Pivoting

Row k

Largest | a ik | Perfute touts

➤ General situation:

Always permute row  $m{k}$  with row  $m{l}$  such that

$$|a_{lk}| = \max_{i=k,\dots,n} |a_{ik}|$$

➤ More 'stable' algorithm.

GvL  $3.\{1,3,5\}$  – Systems

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```
function x = gaussp(A, b)
  function x = guassp(A, b)
  solves A x = b by Gaussian elimination with
  partial pivoting/
\tilde{n} = size(A,1):
A = [A,b]
for k=1:n-1
    [t, ip] = max(abs(A(k:n,k)));
ip = ip+k-1;
%% swap
    temp = A(k,k:n+1) ;
    A(k,k:n+1) = A(ip,k:n+1);
    A(ip,k:n+1) = temp;
     for i=k+1:n
    piv = A(i,k) / A(k,k);
    A(i,k+1:n+1) = A(i,k+1:n+1) - piv*A(k,k+1:n+1);
   end
x = backsolv(A,A(:,n+1));
```

## Pivoting and permutation matrices

- A permutation matrix is a matrix obtained from the identity matrix by permuting its rows
- lacksquare For example for the permutation  $\pi=\{3,1,4,2\}$  we obtain

$$P = egin{pmatrix} 0 & 0 & 1 & 0 \ 1 & 0 & 0 & 0 \ 0 & 0 & 0 & 1 \ 0 & 1 & 0 & 0 \end{pmatrix}$$

Important observation: the matrix PA is obtained from A by permuting its rows with the permutation  $\pi$ 

$$(PA)_{i,:}=A_{\pi(i),:}$$

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Mhat is the matrix PA when

$$P = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 \end{pmatrix} \ A = \begin{pmatrix} 1 & 2 & 3 & 4 \\ 5 & 6 & 7 & 8 \\ 9 & 0 & -1 & 2 \\ -3 & 4 & -5 & 6 \end{pmatrix} ?$$

- $\blacktriangleright$  Any permutation matrix is the product of interchange permutations, which only swap two rows of I.
- Notation:  $E_{ij} =$ Identity with rows i and j swapped

**Example:** To obtain  $\pi = \{3, 1, 4, 2\}$  from  $\pi = \{1, 2, 3, 4\}$  – we need to swap  $\pi(2) \leftrightarrow \pi(3)$  then  $\pi(3) \leftrightarrow \pi(4)$  and finally  $\pi(1) \leftrightarrow \pi(2)$ . Hence:

$$P = egin{pmatrix} 0 & 0 & 1 & 0 \ 1 & 0 & 0 & 0 \ 0 & 0 & 0 & 1 \ 0 & 1 & 0 & 0 \end{pmatrix} = E_{1,2} imes E_{3,4} imes E_{2,3}$$

Matlab gives det(A) = -896. What is det(PA)?

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At each step of G.E. with partial pivoting:

$$M_{k+1}E_{k+1}A_k = A_{k+1}$$

where  $E_{k+1}$  encodes a swap of row k+1 with row l>k+1.

Notes: (1)  $E_i^{-1} = E_i$  and (2)  $M_j^{-1} \times E_{k+1} = E_{k+1} \times \tilde{M}_j^{-1}$  for  $k \geq j$ , where  $\tilde{M}_j$  has a permuted Gauss vector:

$$egin{aligned} (I + v^{(j)} e_j^T) E_{k+1} &= E_{k+1} (I + E_{k+1} v^{(j)} e_j^T) \ &\equiv E_{k+1} (I + ilde{v}^{(j)} e_j^T) \ &\equiv E_{k+1} ilde{M}_i \end{aligned}$$

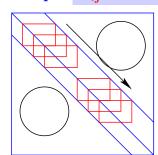
ightharpoonup Here we have used the fact that above row k+1, the permutation matrix  $E_{k+1}$  looks just like an identity matrix.

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# $Special\ case\ of\ banded\ matrices$

- Banded matrices arise in many applications
- lacksquare A has upper bandwidth q if  $a_{ij}=0$  for j-i>q
- ightharpoonup A has lower bandwidth p if  $a_{ij}=0$  for i-j>p



ightharpoonup Simplest case: tridiagonal ightharpoonup p=q=1.

Result:

$$egin{aligned} A_0 &= E_1 M_1^{-1} A_1 \ &= E_1 M_1^{-1} E_2 M_2^{-1} A_2 = E_1 E_2 ilde{M}_1^{-1} M_2^{-1} A_2 \ &= E_1 E_2 ilde{M}_1^{-1} M_2^{-1} E_3 M_3^{-1} A_3 \ &= E_1 E_2 E_3 ilde{M}_1^{-1} ilde{M}_2^{-1} M_3^{-1} A_3 \ &= \dots \ &= E_1 \cdots E_{n-1} \ imes ilde{M}_1^{-1} ilde{M}_2^{-1} ilde{M}_3^{-1} \cdots ilde{M}_{n-1}^{-1} \ ilde{M}_{n-1}^{-1} \ ilde{M}_{n-1}^{-1} \ ilde{M}_{n-1}^{-1} \end{array}$$

➤ In the end

$$PA = LU$$
 with  $P = E_{n-1} \cdots E_1$ 

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First observation: Gaussian elimination (no pivoting) preserves the initial banded form. Consider first step of Gaussian elimination:

- 2. For i = 2 : n Do:
- 3.  $a_{i1} := a_{i1}/a_{11}$  (pivots)
- 4. For j := 2 : n Do :
- 5.  $a_{ij} := a_{ij} a_{i1} * a_{1j}$
- 6. End
- 7. End

GvL 3.{1,3,5} – Systems

GvL 3.{1,3,5} – Systems

▶ If A has upper bandwidth q and lower bandwidth p then so is the resulting [L/U] matrix. ▶ Band form is preserved (induction)

✓ 11 Operation count?

What happens when partial pivoting is used?

If A has lower bandwidth p, upper bandwidth q, and if Gaussian elimination with partial pivoting is used, then the resulting U has upper bandwidth p+q. L has at most p+1 nonzero elements per column (bandedness is lost).

GvL 3.{1,3,5} – Systems

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ightharpoonup Simplest case: tridiagonal ightharpoonup p = q = 1.

Example:

$$A = egin{pmatrix} 1 & 1 & 0 & 0 & 0 \ 2 & 1 & 1 & 0 & 0 \ 0 & 2 & 1 & 1 & 0 \ 0 & 0 & 2 & 1 & 1 \ 0 & 0 & 0 & 2 & 1 \end{pmatrix}$$

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