# solving systems

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# goals for today…

- Identify *why* our basic GE method is “naive”: identify where the errors come from?
    - division by zero, near-zero
- Propose strategies to eliminate the errors
    - partial pivoting, complete pivoting, scaled partial pivoting
- Investigate the cost: does pivoting cost too much?
- Try to answer “How *accurately* can we solve a system with or without pivoting?”
    - Analysis tools: norms, condition number, . . .

# why is our basic ge “naive”?

## Example

$$A = \begin{bmatrix} 0 & 2 & 3 \\ 4 & 5 & 6 \\ 7 & 8 & 9 \end{bmatrix}$$

## Example

$$A = \begin{bmatrix} 1e-10 & 2 & 3 \\ 4 & 5 & 6 \\ 7 & 8 & 9 \end{bmatrix}$$

# the need for pivoting

Solve:

$$A = \begin{bmatrix} 2 & 4 & -2 & -2 \\ 1 & 2 & 4 & -3 \\ -3 & -3 & 8 & -2 \\ -1 & 1 & 6 & -3 \end{bmatrix} \qquad b = \begin{bmatrix} -4 \\ 5 \\ 7 \\ 7 \end{bmatrix}$$

Note that there is nothing ”wrong” with this system. $A$ is full rank. The solution exists and is unique.

Form the augmented system.

$$\left[\begin{array}{rrrr|r} 2 & 4 & -2 & -2 & -4 \\ 1 & 2 & 4 & -3 & 5 \\ -3 & -3 & 8 & -2 & 7 \\ -1 & 1 & 6 & -3 & 7 \end{array}\right]$$

# the need for pivoting

Subtract $1/2$ times the first row from the second row,
add $3/2$ times the first row to the third row,
add $1/2$ times the first row to the fourth row.

The result of these operations is:

$$\left[\begin{array}{cccc|c} 2 & 4 & -2 & -2 & -4 \\ 0 & 0 & 5 & -2 & 7 \\ 0 & 3 & 5 & -5 & 1 \\ 0 & 3 & 5 & -4 & 5 \end{array}\right]$$

The *next* stage of Gaussian elimination will not work because there is a zero in the *pivot* location, $\tilde{a}_{22}$.

# the need for pivoting

Swap second and fourth rows of the augmented matrix.

$$\left[\begin{array}{cccc|c} 2 & 4 & -2 & -2 & -4 \\ 0 & 3 & 5 & -4 & 5 \\ 0 & 3 & 5 & -5 & 1 \\ 0 & 0 & 5 & -2 & 7 \end{array}\right]$$

Continue with elimination: subtract (1 times) row 2 from row 3.

$$\left[\begin{array}{cccc|c} 2 & 4 & -2 & -2 & -4 \\ 0 & 3 & 5 & -4 & 5 \\ 0 & 0 & 0 & -1 & -4 \\ 0 & 0 & 5 & -2 & 7 \end{array}\right]$$

# the need for pivoting

Another zero has appear in the pivot position. Swap row 3 and row 4.

$$\left[\begin{array}{cccc|c} 2 & 4 & -2 & -2 & -4 \\ 0 & 3 & 5 & -4 & 5 \\ 0 & 0 & 5 & -2 & 7 \\ 0 & 0 & 0 & -1 & -4 \end{array}\right]$$

The augmented system is now ready for backward substitution.

# another example

$$\begin{bmatrix} \varepsilon & 1 \\ 1 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 1 \\ 2 \end{bmatrix}$$

## Example

With Naive GE,

$$\begin{bmatrix} \varepsilon & 1 \\ 0 & (1 - \frac{1}{\varepsilon}) \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 1 \\ 2 - \frac{1}{\varepsilon} \end{bmatrix}$$

Solving for $x_1$ and $x_2$ we get

$$x_2 = \frac{2 - 1/\varepsilon}{1 - 1/\varepsilon}$$

$$x_1 = \frac{1 - x_2}{\varepsilon}$$

For $\varepsilon \approx 10^{-20}$, $x_1 \approx 0$, $x_2 \approx 1$

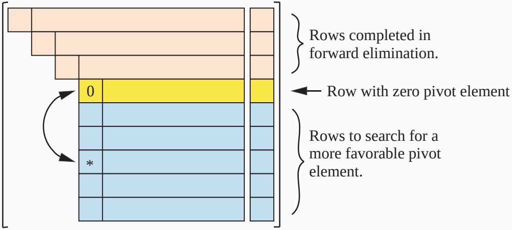
# pivoting strategies

**Partial Pivoting:** Exchange only rows

- Exchanging rows does not affect the order of the $x_i$
- For increased numerical stability, make sure the largest possible pivot element is used. This requires searching in the partial column below the pivot element.
- Partial pivoting is usually sufficient.

# partial pivoting

To avoid division by zero, swap the row having the zero pivot with one of the rows below it.


Rows completed in forward elimination.
0
Row with zero pivot element
*
Rows to search for a more favorable pivot element.

To minimize the effect of roundoff, always choose the row that puts the largest pivot element on the diagonal, i.e., find $i_p$ such that $|a_{i_p,i}| = \max(|a_{k,i}|)$ for $k = i, \ldots, n$

# partial pivoting: usually sufficient, but not always

- Partial pivoting is <u>usually</u> sufficient
- Consider

$$\left[\begin{array}{cc|c} 2 & 2c & 2c \\ 1 & 1 & 2 \end{array}\right]$$

With Partial Pivoting, the first row is the pivot row:

$$\left[\begin{array}{cc|c} 2 & 2c & 2c \\ 0 & 1-c & 2-c \end{array}\right]$$

and for large $c$:

$$\left[\begin{array}{cc|c} 2 & 2c & 2c \\ 0 & -c & -c \end{array}\right]$$

so that $y = 0$ and $x = 1$. (exact is $x = y = 1$)

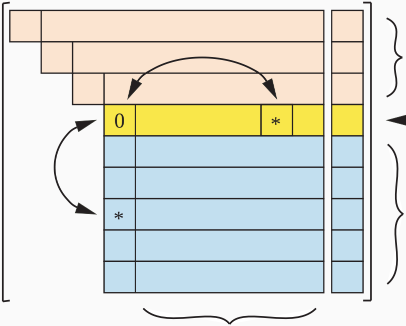
- The pivot is selected as the largest in the column, but it should be the largest <u>relative</u> to the full submatrix.

# more pivoting strategies

**Full (or Complete) Pivoting:** Exchange *both* rows and columns

- Column exchange requires changing the order of the $x_i$
- For increased numerical stability, make sure the largest possible pivot element is used. This requires searching in the pivot row, *and* in all rows below the pivot row, starting the pivot column.
- Full pivoting is less susceptible to roundoff, but the increase in stability comes at a cost of more complex programming (not a problem if you use a library routine) and an increase in work associated with searching and data movement.

# full pivoting



Rows completed in forward elimination.

Row with zero pivot element

Rows to search for a more favorable pivot element.

Columns to search for a more favorable pivot element.

# scaled partial pivoting

We simulate full pivoting by using a scale with partial pivoting.

- pick pivot element as the largest **relative** entry in the column (relative to the other entries in the row)
- do not swap, just keep track of the order of the pivot rows
- call this vector $\ell = [\ell_1, \ldots, \ell_n]$.

# spp process

1. Determine a scale vector **s**. For each row
$$s_i = \max_{1 \leqslant j \leqslant n} |a_{ij}|$$
2. initialize $\ell = [\ell_1, \dots, \ell_n] = [1, \dots, n]$.
3. select row $j$ to be the row with the largest ratio
$$\frac{|a_{\ell_i 1}|}{s_{\ell_i}} \qquad 1 \leqslant i \leqslant n$$
4. swap $\ell_j$ with $\ell_1$ in $\ell$
5. Now we need $n - 1$ multipliers for the first column:
$$m_1 = \frac{a_{\ell_i 1}}{a_{\ell_1 1}}$$
6. So the index to the rows are being swapped, NOT the actual row vectors which would be expensive
7. finally use the multiplier $m_1$ times row $\ell_1$ to subtract from rows $\ell_i$ for $2 \leqslant i \leqslant n$

# spp process continued

1. For the second column in forward elimination, we select row $j$ that yields the largest ratio of

$$\frac{|a_{\ell_i,2}|}{s_{\ell_i}} \qquad 2 \leqslant i \leqslant n$$

2. swap $\ell_j$ with $\ell_2$ in $\ell$
3. Now we need $n - 2$ multipliers for the second column:

$$m_2 = \frac{a_{\ell_i,2}}{a_{\ell_2 2}}$$

4. finally use the multiplier $m_2$ times row $\ell_2$ to subtract from rows $\ell_i$ for $3 \leqslant i \leqslant n$
5. the process continues for row $k$
6. note: scale factors are *not* updated

# an example

Consider

$$\begin{bmatrix} 2 & 4 & -2 \\ 1 & 3 & 4 \\ 5 & 2 & 0 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 6 \\ -1 \\ 2 \end{bmatrix}$$

# back substitution. . .

1. The first equation corresponds to the last index $\ell_n$:

$$a_{\ell_n n} x_n = b_{\ell_n} \;\Rightarrow\; x_n = \frac{b_{\ell_n}}{a_{\ell_n n}}$$

2. The second equation corresponds to the second to last index $\ell_{n-1}$:

$$x_{n-1} = \frac{1}{a_{\ell_{n-1} n-1}} \left( b_{\ell_{n-1}} - a_{\ell_{n-1} n} x_n \right)$$

# the algorithms

Listing 1: (forward) GE with SPP

```
Initialize $\ell = [1, \ldots, n]$
Set **s** to be the max of rows
for $k = 1$ to $n$
  $rmax = 0$
  for $i = k$ to $n$
    $r = |a_{\ell_i k} / s_{\ell_i}|$
    if($r > rmax$)
      $rmax = r$
      $j = i$
  end
  swap $\ell_j$ and $\ell_k$
  for $i = k + 1$ to $n$
    $xmult = a_{\ell_i k} / a_{\ell_k k}$
    $a_{\ell_{ik}} = xmult$
    for $j = k + 1$ to $n$
      $a_{\ell_i j} = a_{\ell_i j} - xmult \cdot a_{\ell_k j}$
    end
  end
end
```

# the algorithms

Note: the multipliers are stored in the location $a_{\ell_i k}$ in the text

Listing 2: (back solve) GE with SPP

```
for $k = 1$ to $n - 1$
    for $i = k + 1$ to $n$
        $b_{\ell_i} = b_{\ell_i} - a_{\ell_i k} b_{\ell_k}$
    end
end
$x_n = b_{\ell_n} / a_{\ell_n n}$
for $i = n - 1$ down to 1
    $sum = b_{\ell_i}$
    for $j = i + 1$ to $n$
        $sum = sum - a_{\ell_i j} x_j$
    end
end
```

# geometric interpretation of singularity

Consider a 2 × 2 system describing two lines that intersect

$$\begin{aligned} y &= -2x + 6 \\ y &= \ \ \frac{1}{2}x + 1 \end{aligned}$$

The matrix form of this equation is

$$\begin{bmatrix} 2 & 1 \\ -1/2 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 6 \\ 1 \end{bmatrix}$$

The equations for two **parallel** but **not intersecting** lines are

$$\begin{bmatrix} 2 & 1 \\ 2 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 6 \\ 5 \end{bmatrix}$$

Here the coefficient matrix is singular ($\mathrm{rank}(A) = 1$), and the system is inconsistent

# geometric interpretation of singularity

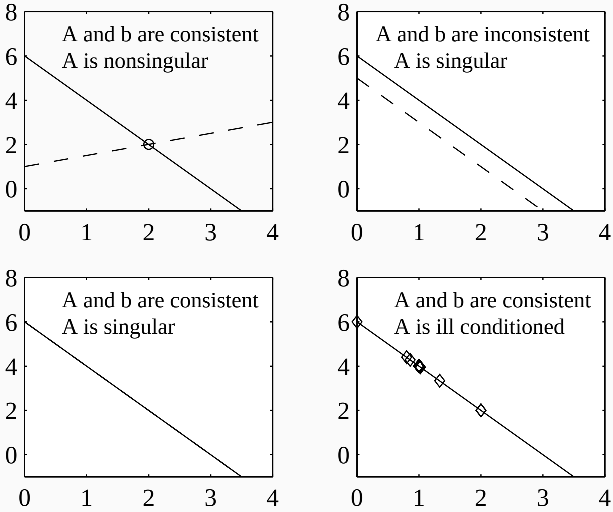
The equations for two **parallel** and **coincident** lines are

$$\begin{bmatrix} 2 & 1 \\ 2 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 6 \\ 6 \end{bmatrix}$$

The equations for two **nearly parallel** lines are

$$\begin{bmatrix} 2 & 1 \\ 2+\delta & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 6 \\ 6+\delta \end{bmatrix}$$

# geometric interpretation of singularity



# effect of perturbations to *b*

Consider the solution of a $2 \times 2$ system where

$$b = \begin{bmatrix} 1 \\ 2/3 \end{bmatrix}$$

One expects that the *exact* solutions to

$$Ax = \begin{bmatrix} 1 \\ 2/3 \end{bmatrix} \qquad \text{and} \qquad Ax = \begin{bmatrix} 1 \\ 0.6667 \end{bmatrix}$$

will be different. Should these solutions be a **lot different** or a **little different**?

# norms

Vectors:

$$\|x\|_p = \left(|x_1|^p + |x_2|^p + \ldots + |x_n|^p\right)^{1/p}$$

$$\|x\|_1 = |x_1| + |x_2| + \ldots + |x_n| = \sum_{i=1}^{n} |x_i|$$

$$\|x\|_\infty = \max\left(|x_1|, |x_2|, \ldots, |x_n|\right) = \max_i\left(|x_i|\right)$$

Matrices:

$$\|A\| = \max_{x \neq 0} \frac{\|Ax\|}{\|x\|}$$

$$\|A\|_p = \max_{x \neq 0} \frac{\|Ax\|_p}{\|x\|_p}$$

$$\|A\|_1 = \max_{1 \leqslant j \leqslant n} \sum_{i=1}^{m} |a_{ij}|$$

$$\|A\|_\infty = \max_{1 \leqslant i \leqslant m} \sum_{j=1}^{n} |a_{ij}|$$

# effect of perturbations to $b$

Perturb $b$ with $\delta b$ such that

$$\frac{\|\delta b\|}{\|b\|} \ll 1,$$

The perturbed system is

$$A(x + \delta x_b) = b + \delta b$$

The perturbations satisfy

$$A\delta x_b = \delta b$$

Analysis shows (see next two slides for proof) that

$$\frac{\|\delta x_b\|}{\|x\|} \leqslant \|A\|\|A^{-1}\|\frac{\|\delta b\|}{\|b\|}$$

Thus, the effect of the perturbation is small *only if* $\|A\|\|A^{-1}\|$ is small.

$$\frac{\|\delta x_b\|}{\|x\|} \ll 1 \quad \text{only if} \quad \|A\|\|A^{-1}\| \sim 1$$

# effect of perturbations to $b$ (proof)

Let $x + \delta x_b$ be the *exact* solution to the perturbed system

$$A(x + \delta x_b) = b + \delta b \tag{1}$$

Expand

$$Ax + A\delta x_b = b + \delta b$$

Subtract $Ax$ from left side and $b$ from right side since $Ax = b$

$$A\delta x_b = \delta b$$

Left multiply by $A^{-1}$

$$\delta x_b = A^{-1}\delta b \tag{2}$$

# effect of perturbations to $b$ (proof, p. 2)

Take norm of equation (2)

$$\|\delta x_b\| = \|A^{-1}\,\delta b\|$$

Applying consistency requirement of matrix norms

$$\|\delta x\| \leqslant \|A^{-1}\|\|\delta b\| \tag{3}$$

Similarly, $Ax = b$ gives $\|b\| = \|Ax\|$, and

$$\|b\| \leqslant \|A\|\|x\| \tag{4}$$

Rearrangement of equation (4) yields

$$\frac{1}{\|x\|} \leqslant \frac{\|A\|}{\|b\|} \tag{5}$$

# effect of perturbations to $b$ (proof)

Multiply Equation (4) by Equation (3) to get

$$\frac{\|\delta x_b\|}{\|x\|} \leqslant \|A\|\|A^{-1}\|\frac{\|\delta b\|}{\|b\|} \tag{6}$$

**Summary:**

If $x+\delta x_b$ is the *exact* solution to the perturbed system

$$A(x+\delta x_b) = b + \delta b$$

then

$$\frac{\|\delta x_b\|}{\|x\|} \leqslant \|A\|\|A^{-1}\|\frac{\|\delta b\|}{\|b\|}$$

# effect of perturbations to *a*

Perturb $A$ with $\delta A$ such that

$$\frac{\|\delta A\|}{\|A\|} \ll 1,$$

The perturbed system is

$$(A + \delta A)(x + \delta x_A) = b$$

Analysis shows that

$$\frac{\|\delta x_A\|}{\|x + \delta x_A\|} \leqslant \|A\|\|A^{-1}\| \frac{\|\delta A\|}{\|A\|}$$

Thus, the effect of the perturbation is small *only if* $\|A\|\|A^{-1}\|$ is small.

$$\frac{\|\delta x_A\|}{\|x + \delta x_A\|} \ll 1 \quad \text{only if} \quad \|A\|\|A^{-1}\| \sim 1$$

# effect of perturbations to both *a* and *b*

Perturb both $A$ with $\delta A$ and $b$ with $\delta b$ such that

$$\frac{\|\delta A\|}{\|A\|} \ll 1 \quad \text{and} \quad \frac{\|\delta b\|}{\|b\|} \ll 1$$

The perturbation satisfies

$$(A + \delta A)(x + \delta x) = b + \delta b$$

Analysis shows that

$$\frac{\|\delta x\|}{\|x + \delta x\|} \quad \leqslant \quad \frac{\|A\|\|A^{-1}\|}{1 - \|A\|\|A^{-1}\|\frac{\|\delta A\|}{\|A\|}} \left[\frac{\|\delta A\|}{\|A\|} + \frac{\|\delta b\|}{\|b\|}\right]$$

Thus, the effect of the perturbation is small *only if* $\|A\|\|A^{-1}\|$ is small.

$$\frac{\|\delta x\|}{\|x + \delta x\|} \ll 1 \quad \text{only if} \quad \|A\|\|A^{-1}\| \sim 1$$

# condition number of *a*

The **condition number**

$$\kappa(A) \equiv \|A\|\|A^{-1}\|$$

indicates the sensitivity of the solution to perturbations in $A$ and $b$. The condition number can be measured with any $p$-norm.

The condition number is always in the range

$$1 \leqslant \kappa(A) \leqslant \infty$$

- $\kappa(A)$ *is a mathematical property of* $A$
- *Any algorithm will produce a solution that is sensitive to perturbations in* $A$ *and* $b$ *if* $\kappa(A)$ *is large.*
- *In exact math a matrix is either singular or non-singular.* $\kappa(A) = \infty$ *for a singular matrix*
- $\kappa(A)$ *indicates how close* $A$ *is to being numerically singular.*
- *A matrix with large* $\kappa$ *is said to be* ***ill-conditioned***

# computational stability

**In Practice**, applying Gaussian elimination with partial pivoting and back substitution to $Ax = b$ gives the **exact solution**, $\hat{x}$, to the **nearby problem**

$$(A + E)\hat{x} = b \quad \text{where} \quad \|E\|_\infty \leqslant \varepsilon_m \|A\|_\infty$$

> *Gaussian elimination with partial pivoting and back substitution "gives exactly the right answer to nearly the right question."*
>
> *— Trefethen and Bau*

# computational stability

An algorithm that gives the exact answer to a problem that is near to the original problem is said to be **backward stable**. Algorithms that are not backward stable will tend to amplify roundoff errors present in the original data. As a result, the solution produced by an algorithm that is not backward stable will not necessarily be the solution to a problem that is close to the original problem.

Gaussian elimination without partial pivoting is *not* backward stable for arbitrary $A$.

If $A$ is symmetric and positive definite, then Gaussian elimination without pivoting in backward stable.

# the residual

Let $\hat{x}$ be the numerical solution to $Ax = b$. $\hat{x} \neq x$ ($x$ is the exact solution) because of roundoff.

The **residual** measures how close $\hat{x}$ is to satisfying the original equation

$$r = b - A\hat{x}$$

It is not hard to show that

$$\frac{\|\hat{x} - x\|}{\|\hat{x}\|} \leqslant \kappa(A)\frac{\|r\|}{\|b\|}$$

Small $\|r\|$ does not guarantee a small $\|\hat{x} - x\|$.

If $\kappa(A)$ is large the $\hat{x}$ returned by Gaussian elimination and back substitution (or any other solution method) is *not* guaranteed to be anywhere near the true solution to $Ax = b$.

# rules of thumb

- Applying Gaussian elimination with partial pivoting and back substitution to $Ax = b$ yields a numerical solution $\hat{x}$ such that the residual vector $r = b - A\hat{x}$ is small *even if* the $\kappa(A)$ is large.
- If $A$ and $b$ are stored to machine precision $\varepsilon_m$, the numerical solution to $Ax = b$ by any variant of Gaussian elimination is correct to $d$ digits where

$$d = |\log_{10}(\varepsilon_m)| - \log_{10}(\kappa(A))$$

# rules of thumb

$$d = |\log_{10}(\varepsilon_m)| - \log_{10}(\kappa(A))$$

**Example:**

Computations have $\varepsilon_m \approx 2.2 \times 10^{-16}$ in IEEE double precision. For a system with $\kappa(A) \sim 10^{10}$ the elements of the solution vector will have

$$\begin{aligned} d &= |\log_{10}(2.2 \times 10^{-16})| - \log_{10}\left(10^{10}\right) \\ &= 16 - 11 \\ &= 5 \end{aligned}$$

correct (decimal) digits

# summary of limits to numerical solution of $ax = b$

1. $\kappa(A)$ indicates how close $A$ is to being numerically singular
2. If $\kappa(A)$ is "large", $A$ is **ill-conditioned** and *even the best* numerical algorithms will produce a solution, $\hat{x}$ that cannot be guaranteed to be close to the true solution, $x$
3. In practice, Gaussian elimination with partial pivoting and back substitution produces a solution with a small residual

   $$r = b - A\hat{x}$$

   *even if* $\kappa(A)$ is large.