More on Systems of Linear Equations

Iñaki Rañó

The Mærsk Mc Kinney Møller Institute

2021

Contents

Solving Systems of Linear Equations (Review)

Systems of linear equations of the form: $A\mathbf{v} = \mathbf{b}$

- Can be seen as the intersection of planes/hyperplanes
- Cramer's rule
- Back substitution (for A upper triangular)
- Gaussian Elimination + back substitution
  - Augmented matrix $\tilde{A} = [A|\mathbf{b}]$
  - Solution or not depends on ranks of A, $\tilde{A}$ and number of unknowns
- If A has an inverse (i.e. A is square and $|A| \neq 0$) A^{-1} then:

$$A^{-1}A\mathbf{x} = A^{-1}\mathbf{b} \qquad \rightarrow \qquad \mathbf{x} = A^{-1}\mathbf{b}$$

  - Gaussian elimination is more efficient than calculating A^{-1}
  - Calculating A^{-1} is useful for other problems

Gaussian Elimination Review

Goal: To turn matrix $\tilde{A}$ into upper triangular (row echelon form)

Allowed operations:

- Swap two rows
- Multiply one row by a number different than zero
- Substitute row 'i' by row 'i' plus another multiplied by a number

The second rule is not really necessary to make the matrix upper triangular (it is just convenient sometimes to have 1 as first non-zero entry in the row)

Gaussian Elimination Procedure Review

While there are non-zero columns and rows:

1 Make sure entry row 1, column 1 is not zero (swap rows 1 and $i > 1$ if necessary)

2 Take entry row 1, column 1 and use last rule to make all zeros under it (from row 2 to last row)

3 Make sure entry row 2, column 2 is not zero (swap rows 2 and $i > 2$ if necessary)

4 Take entry row 2, column 2 and use last rule to make all zeros under it (from row 3 to last row)

$\vdots$ $\quad \vdots$

k_0 Make sure entry row 'k', column 'k' is not zero (swap rows 'k' and $i > k$ if necessary)

k_1 Move to entry row i, column i and use last rule to make all zeros under it

Gaussian Elimination as an Algorithm

For a matrix A of size $m \times n$

- The steps to do Gaussian elimination can be easily automated in a computer
- The current entry (row 'k', column 'k') is called **pivot**
- Take as pivot row 'k', column 'k (if not zero, swap otherwise if possible) for $k = 1, 2, \cdots, min(m, n)$ and turn all entries under it to zero (row $k+1, k+2, \cdots, m$, column 'k')

Gaussian Elimination Algorithm

```
Input: Matrix A of size m × n
Output: Matrix A in upper triangular (row echelon) form
pivot_row ← 1                                              ▷ Initial pivot
pivot_col ← 1
while pivot_row ≤ m and pivot_col ≤ n do
    idx_max ← index_of_max_abs(A, pivot_row, pivot_col)    ▷ See later
    if A(idx_max, pivot_col) = 0 then                      ▷ 'Column' of zeros
        pivot_col ← pivot_col + 1                          ▷ Skip column
    else
        A ← swap_rows(A, pivot_row, idx_max)               ▷ See later
        for i = pivot_row + 1, ··· , m do                  ▷ Zero entries under pivot
            α ← A(i,pivot_col) / A(pivot_row,pivot_col)
            A(i, pivot_col) ← 0                            ▷ Avoid numerical errors
            for j = pivot_col + 1, ··· , n do              ▷ Operate whole row
                A(i, j) ← A(i, j) − αA(pivot_row, j)
            end for
        end for
        pivot_row ← pivot_row + 1                          ▷ Next pivot
        pivot_col ← pivot_col + 1
    end if
end while
```

Gaussian Elimination Algorithm (ii)

The Function $index\_of\_max\_abs()$ finds the index of the largest absolute value of A from $pivot\_row$ to the end of the $pivot\_col$ column.

Input: Matrix A of size $m \times n$, $pivot\_row$, $pivot\_col$
Output: Row number: idx_max
$idx\_max \leftarrow pivot\_row$
for $i = pivot\_row + 1, \cdots, m$ **do**
  if $abs(A(i, pivot\_col)) > abs(A(idx\_max, pivot\_col))$ **then**
    $idx\_max \leftarrow i$
  end if
end for

Notes:

- Check only under the pivot
- Any non-zero entry should work (doesn't need to be the absolute maximum)
- Function might exist in some programming languages

Gaussian Elimination Algorithm (iii)

The Function *swap_rows*() swaps two rows in the matrix A.

Input: Matrix A of size $m \times n$, $row1$, $row2$
Output: New matrix A of size $m \times n$,
for $i = 1, \cdots, n$ **do**
    $temp \leftarrow A(row1, i)$
    $A(row1, i) \leftarrow A(row2, i)$
    $A(row2, i) \leftarrow temp$
end for

- Need to swap the whole row? (not really, but simpler)
- Temporary copy of one entry
- Programming language arrays start on '0' or '1'? (applies to Gaussian algorithm too)

Interpretation of Linear Equations

In a linear system of equations $A\mathbf{x} = \mathbf{b}$ each equation (matrix row)

$$a_{i1}x_1 + a_{i2}x_2 + \cdots + a_{in}x_n = b_i$$

corresponds to a hyperplane in $\mathbb{R}^n$ (line/plane in 2D/3D).

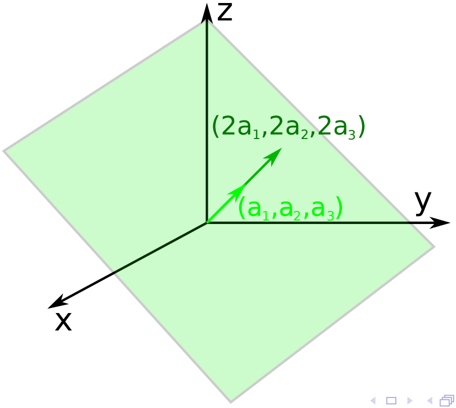
We define the vector $\mathbf{a}_i = [a_{i1}, a_{i2}, \cdots, a_{in}]$ in $\mathbb{R}^n$ and the equation becomes $\mathbf{a}_i \cdot \mathbf{x} = b_i$ (dot product of $\mathbf{a}_i$ and $\mathbf{x}$)

- If $b_i = 0$ the equation is: $\mathbf{a}_i \cdot \mathbf{x} = 0$.
  - Vectors $\mathbf{a}_i$ and $\mathbf{x}$ are perpendicular
  - Points '$\mathbf{x}$' in the plane when 'perpendicular' to $\mathbf{a}_i$
  - $\mathbf{a}_i$ is called **normal vector**
- If $b_i \neq 0$ the equation is: $\mathbf{a}_i \cdot \mathbf{x} = b_i$.
  - Dot product is the projection of vector $\mathbf{x}$ along direction $\mathbf{a}_i$
  - If $|\mathbf{a}_i| = 1$ then b_i is the distance from the plane to the origin $\mathbf{O} = [0, 0, \cdots, 0]$ (perpendicular projection)
  - In general $b_i = |\mathbf{a}_i|d$ with 'd' distance from the plane to the origin (if $d = 0$ previous case)

Geometrical Interpretation of the Scaling Rule (R^3)

Assuming $b_i = 0$, in Gaussian elimination multiplying a row by $\alpha \neq 0$ means scaling $\mathbf{a}_i$.

- Normal vector $\mathbf{a}_i$ perpendicular to the plane
- Vector $\alpha\mathbf{a}_i$ has the same direction (remains perpendicular)
- Still 'true' for $b_i \neq 0$ and $\mathbb{R}^n$



Interpretation of Linear Equations (cont)

In a linear system of equations $A\mathbf{x} = \mathbf{b}$ considering two equation (matrix rows) simultaneously

$$a_{i1}x_1 + a_{i2}x_2 + \cdots + a_{in}x_n = b_i$$
$$a_{j1}x_1 + a_{j2}x_2 + \cdots + a_{jn}x_n = b_j$$

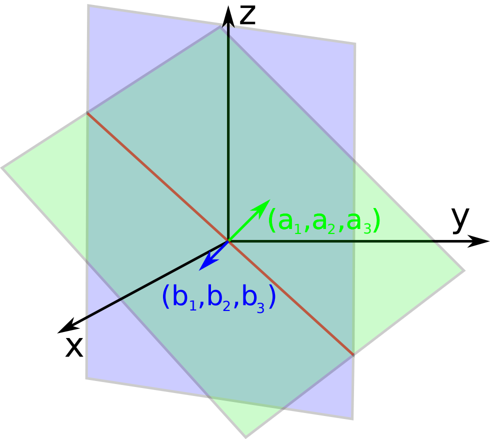
corresponds to the intersection of hyperplanes in $\mathbb{R}^n$ (point/line in 2D/3D).

Defining the vectors as before $\mathbf{a}_i$ and $\mathbf{a}_j$ equation $\mathbf{a}_i \cdot \mathbf{x} = b_i$ can be replaced by $\mathbf{a}_i \cdot \mathbf{x} + \alpha\mathbf{a}_j \cdot \mathbf{x} = (\mathbf{a}_i + \alpha\mathbf{a}_j) \cdot \mathbf{x} = b_i + \alpha b_j$

- If $b_i = b_j = 0$ substitute $\mathbf{a}_i \cdot \mathbf{x} = 0$ by a hyperplane with normal $\mathbf{a}_i + \alpha\mathbf{a}_j$ (linear combination of $\mathbf{a}_i$ and $\mathbf{a}_j$)
  - That hyperplane has the same intersection with $\mathbf{a}_j \cdot \mathbf{x} = 0$ as $\mathbf{a}_i \cdot \mathbf{x} = 0$
  - 'Rotation' of $\mathbf{a}_i$ in 3D
- If $b_i \neq 0$and $b_j \neq 0$ the hyperplane has the same intersection

Geometrical Interpretation of the Combination Rule (R^3)

- Intersection of two planes is a line (except when $\mathbf{a} = k\mathbf{b}$)
- Plane $(\mathbf{a} + \alpha\mathbf{b}) \cdot \mathbf{v} = 0$ is a plane 'rotated' along the intersection line



Gauss-Jordan Elimination

An extension of the Gauss Elimination algorithm that allows to obtain the inverse (A^{-1}) of a square matrix A (if $|A| \neq 0$).

Augmented matrix:

$$\tilde{A} = \left[\begin{array}{cccc|cccc} a_{11} & a_{12} & \cdots & a_{1n} & 1 & 0 & \cdots & 0 \\ a_{21} & a_{22} & \cdots & a_{2n} & 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nn} & 0 & 0 & \cdots & 1 \end{array}\right]$$

Augment the matrix A with the $n \times n$ identity matrix

- Make the submatrix A of $\tilde{A}$ upper triangular
- Make the submatrix A of $\tilde{A}$ diagonal
- Make the submatrix A of $\tilde{A}$ the identity matrix
- The submatrix on the right is the inverse of A: A^{-1}

Gauss-Jordan Elimination Example

Using Gauss-Jordan elimination obtain the inverse of the matrix:

$$A = \begin{bmatrix} -1 & 1 & 2 \\ 3 & -1 & 1 \\ -1 & 3 & 4 \end{bmatrix}$$

- Same rules apply:
  - Row swap
  - Row scaling
  - Row combination
- Steps:
  1. Build augmented matrix $\tilde{A}$ adding the identity
  2. Convert to upper triangular
  3. Convert to diagonal (no row swapping)
  4. Convert to identity (only scaling)
- Maybe check if the inverse exists (product of diagonal entries of the upper triangular matrix)

Gauss-Jordan Elimination Example (Upper Triangular A)

Row 2 $+3\times$Row 1

$$\tilde{A} = \left[\begin{array}{ccc|ccc} -1 & 1 & 2 & 1 & 0 & 0 \\ 3 & -1 & 1 & 0 & 1 & 0 \\ -1 & 3 & 4 & 0 & 0 & 1 \end{array}\right] \rightarrow \left[\begin{array}{ccc|ccc} -1 & 1 & 2 & 1 & 0 & 0 \\ 0 & 2 & 7 & 3 & 1 & 0 \\ -1 & 3 & 4 & 0 & 0 & 1 \end{array}\right]$$

Gauss-Jordan Elimination Example (Upper Triangular A)

Row 3 $-$Row 1

$$\tilde{A} = \left[\begin{array}{ccc|ccc} -1 & 1 & 2 & 1 & 0 & 0 \\ 3 & -1 & 1 & 0 & 1 & 0 \\ -1 & 3 & 4 & 0 & 0 & 1 \end{array}\right] \rightarrow \left[\begin{array}{ccc|ccc} -1 & 1 & 2 & 1 & 0 & 0 \\ 0 & 2 & 7 & 3 & 1 & 0 \\ -1 & 3 & 4 & 0 & 0 & 1 \end{array}\right] \rightarrow$$

$$\rightarrow \left[\begin{array}{ccc|ccc} -1 & 1 & 2 & 1 & 0 & 0 \\ 0 & 2 & 7 & 3 & 1 & 0 \\ 0 & 2 & 2 & -1 & 0 & 1 \end{array}\right]$$

Gauss-Jordan Elimination Example (Upper Triangular A)

Row 3 $-$Row 2

$$\tilde{A} = \left[\begin{array}{ccc|ccc} -1 & 1 & 2 & 1 & 0 & 0 \\ 3 & -1 & 1 & 0 & 1 & 0 \\ -1 & 3 & 4 & 0 & 0 & 1 \end{array}\right] \rightarrow \left[\begin{array}{ccc|ccc} -1 & 1 & 2 & 1 & 0 & 0 \\ 0 & 2 & 7 & 3 & 1 & 0 \\ 0 & 2 & 2 & -1 & 0 & 1 \end{array}\right] \rightarrow$$

$$\rightarrow \left[\begin{array}{ccc|ccc} -1 & 1 & 2 & 1 & 0 & 0 \\ \color{red}0 & \color{red}2 & \color{red}7 & \color{red}3 & \color{red}1 & \color{red}0 \\ \color{red}0 & \color{red}0 & \color{red}{-5} & \color{red}{-4} & \color{red}{-1} & \color{red}1 \end{array}\right]$$

We reached the point where the submatrix A is upper triangular, but we have to continue to make it diagonal.

Gauss-Jordan Elimination Example (Diagonal A)

Row 2 $+\frac{7}{5}\times$Row 3

$$\tilde{A} = \left[\begin{array}{ccc|ccc} -1 & 1 & 2 & 1 & 0 & 0 \\ 3 & -1 & 1 & 0 & 1 & 0 \\ -1 & 3 & 4 & 0 & 0 & 1 \end{array}\right] \rightarrow \left[\begin{array}{ccc|ccc} -1 & 1 & 2 & 1 & 0 & 0 \\ 0 & 2 & 7 & 3 & 1 & 0 \\ 0 & 0 & -5 & -4 & -1 & 1 \end{array}\right] \rightarrow$$

$$\rightarrow \left[\begin{array}{ccc|ccc} -1 & 1 & 2 & 1 & 0 & 0 \\ 0 & 2 & 0 & -\frac{13}{5} & -\frac{2}{5} & \frac{7}{5} \\ 0 & 0 & -5 & -4 & -1 & 1 \end{array}\right]$$

Gauss-Jordan Elimination Example (Diagonal A)

Row 1 $-\frac{1}{2}$Row 2

$$\tilde{A} = \left[\begin{array}{ccc|ccc} -1 & 1 & 2 & 1 & 0 & 0 \\ 3 & -1 & 1 & 0 & 1 & 0 \\ -1 & 3 & 4 & 0 & 0 & 1 \end{array}\right] \rightarrow \left[\begin{array}{ccc|ccc} -1 & 1 & 2 & 1 & 0 & 0 \\ 0 & 2 & 0 & -\frac{13}{5} & -\frac{2}{5} & \frac{7}{5} \\ 0 & 0 & -5 & -4 & -1 & 1 \end{array}\right] \rightarrow$$

$$\rightarrow \left[\begin{array}{ccc|ccc} -1 & 0 & 2 & \frac{23}{10} & \frac{2}{10} & -\frac{7}{10} \\ 0 & 2 & 0 & -\frac{13}{5} & -\frac{2}{5} & \frac{7}{5} \\ 0 & 0 & -5 & -4 & -1 & 1 \end{array}\right]$$

Gauss-Jordan Elimination Example (Diagonal A)

Row 1 $+\frac{2}{5}$Row 3

$$\tilde{A} = \left[\begin{array}{ccc|ccc} -1 & 1 & 2 & 1 & 0 & 0 \\ 3 & -1 & 1 & 0 & 1 & 0 \\ -1 & 3 & 4 & 0 & 0 & 1 \end{array}\right] \rightarrow \left[\begin{array}{ccc|ccc} -1 & 0 & 2 & \frac{23}{10} & \frac{1}{5} & -\frac{7}{10} \\ 0 & 2 & 0 & -\frac{13}{5} & -\frac{2}{5} & \frac{7}{5} \\ 0 & 0 & -5 & -4 & -1 & 1 \end{array}\right]$$

$$\rightarrow \left[\begin{array}{ccc|ccc} -1 & 0 & 0 & \frac{7}{10} & -\frac{1}{5} & -\frac{3}{10} \\ 0 & 2 & 0 & -\frac{13}{5} & -\frac{2}{5} & \frac{7}{5} \\ 0 & 0 & -5 & -4 & -1 & 1 \end{array}\right]$$

Now the submatrix A is diagonal, but it should be the identity matrix.

Gauss-Jordan Elimination Example (Identity A)

Row 1 $\rightarrow -1\times$Row 1

$$\tilde{A} = \left[\begin{array}{ccc|ccc} -1 & 1 & 2 & 1 & 0 & 0 \\ 3 & -1 & 1 & 0 & 1 & 0 \\ -1 & 3 & 4 & 0 & 0 & 1 \end{array}\right] \rightarrow \left[\begin{array}{ccc|ccc} -1 & 0 & 0 & \frac{7}{10} & -\frac{1}{5} & -\frac{3}{10} \\ 0 & 2 & 0 & -\frac{13}{5} & -\frac{2}{5} & \frac{7}{5} \\ 0 & 0 & -5 & -4 & -1 & 1 \end{array}\right]$$

$$\rightarrow \left[\begin{array}{ccc|ccc} \color{red}{1} & \color{red}{0} & \color{red}{0} & \color{red}{-\frac{7}{10}} & \color{red}{\frac{1}{5}} & \color{red}{\frac{3}{10}} \\ 0 & 2 & 0 & -\frac{13}{5} & -\frac{2}{5} & \frac{7}{5} \\ 0 & 0 & -5 & -4 & -1 & 1 \end{array}\right]$$

Gauss-Jordan Elimination Example (Identity A)

Row 2 $\rightarrow \frac{1}{2} \times$Row 2

$$\tilde{A} = \left[\begin{array}{ccc|ccc} -1 & 1 & 2 & 1 & 0 & 0 \\ 3 & -1 & 1 & 0 & 1 & 0 \\ -1 & 3 & 4 & 0 & 0 & 1 \end{array}\right] \rightarrow \left[\begin{array}{ccc|ccc} 1 & 0 & 0 & -\frac{7}{10} & \frac{1}{5} & \frac{3}{10} \\ 0 & 2 & 0 & -\frac{13}{5} & -\frac{2}{5} & \frac{7}{5} \\ 0 & 0 & -5 & -4 & -1 & 1 \end{array}\right]$$

$$\rightarrow \left[\begin{array}{ccc|ccc} 1 & 0 & 0 & -\frac{7}{10} & \frac{1}{5} & \frac{3}{10} \\ 0 & 1 & 0 & -\frac{13}{10} & -\frac{2}{10} & \frac{7}{10} \\ 0 & 0 & -5 & -4 & -1 & 1 \end{array}\right]$$

Gauss-Jordan Elimination Example (Identity A)

Row 3 $\rightarrow -\frac{1}{5}\times$Row 3

$$\tilde{A} = \left[\begin{array}{ccc|ccc} -1 & 1 & 2 & 1 & 0 & 0 \\ 3 & -1 & 1 & 0 & 1 & 0 \\ -1 & 3 & 4 & 0 & 0 & 1 \end{array}\right] \rightarrow \left[\begin{array}{ccc|ccc} 1 & 0 & 0 & -\frac{7}{10} & \frac{1}{5} & \frac{3}{10} \\ 0 & 1 & 0 & -\frac{13}{10} & -\frac{1}{5} & \frac{7}{10} \\ 0 & 0 & -5 & -4 & -1 & 1 \end{array}\right]$$

$$\rightarrow \left[\begin{array}{ccc|ccc} 1 & 0 & 0 & -\frac{7}{10} & \frac{1}{5} & \frac{3}{10} \\ 0 & 1 & 0 & -\frac{13}{10} & -\frac{1}{5} & \frac{7}{10} \\ {\color{red}0} & {\color{red}0} & {\color{red}1} & {\color{red}\frac{4}{5}} & {\color{red}\frac{1}{5}} & {\color{red}-\frac{1}{5}} \end{array}\right]$$

Gauss-Jordan Elimination Example: A^{-1}

$$\tilde{A} = \left[\begin{array}{ccc|ccc} -1 & 1 & 2 & 1 & 0 & 0 \\ 3 & -1 & 1 & 0 & 1 & 0 \\ -1 & 3 & 4 & 0 & 0 & 1 \end{array}\right] \to \left[\begin{array}{ccc|ccc} 1 & 0 & 0 & -\frac{7}{10} & \frac{1}{5} & \frac{3}{10} \\ 0 & 1 & 0 & -\frac{13}{10} & -\frac{1}{5} & \frac{7}{10} \\ 0 & 0 & 1 & \frac{4}{5} & \frac{1}{5} & -\frac{1}{5} \end{array}\right]$$

Therefore the inverse of A is:

$$A^{-1} = \begin{bmatrix} -\frac{7}{10} & \frac{1}{5} & \frac{3}{10} \\ -\frac{13}{10} & -\frac{1}{5} & \frac{7}{10} \\ \frac{4}{5} & \frac{1}{5} & -\frac{1}{5} \end{bmatrix}$$

Gauss-Jordan Elimination Algorithm

Apply Gauss elimination part to $\tilde{A}$ (size $n \times (2n)$) and then:

$pivot \leftarrow n$ ▷ Initial pivot
while $pivot >= 1$ **do**
  if $A(pivot, pivot) = 0$ **then** ▷ Pivot is zero
    Error(Singular Matrix)
  else
    for $i = pivot - 1, \cdots, 1$ **do** ▷ Zero entries over pivot
      $\alpha \leftarrow \frac{A(i,pivot)}{A(pivot,pivot)}$
      $A(i, pivot) \leftarrow 0$ ▷ Avoid numerical errors
      for $j = pivot + 1, \cdots, 2n$ **do** ▷ Operate whole row
        $A(i, j) \leftarrow A(i, j) - \alpha A(pivot, j)$
      end for
    end for
    $\alpha = \frac{1}{A(pivot,pivot)}$
    for $j = 1, \cdots, 2n$ **do** ▷ Scale row for identity
      $A(pivot, j) \leftarrow \alpha A(pivot, j)$
    end for
    $pivot \leftarrow pivot - 1$ ▷ Next pivot
  end if
end while

Notes on Gauss-Jordan Elimination Algorithm

- **First apply Gauss elimination** to $\tilde{A}$ (see corresponding algorithm)
- Last slide **only** second part of the algorithm
- Inverse A^{-1} must be taken from $\tilde{A}$ (submatrix)
- If one diagonal entry in the upper triangular matrix is zero the original matrix A has no inverse (singular)

Back to Linear Systems of Equations

A linear system of 'n' equations in 'n' variables $A\mathbf{x} = \mathbf{b}$ can be solved using Gauss-Jordan elimination to obtain A^{-1} and the solution is then $x = A^{-1}b$ (matrix vector product).

Typically if the system $A\mathbf{x} = \mathbf{b}$ has 'm' equations in 'n' variables one can do:

- If $m > n$ (e.g. linear regression) multiplying both sides by A^T
$$A^T A\mathbf{x} = A^T b$$
where $A^T A$ is an $n \times n$ matrix (hopefully not singular), and multiplying both sides by $(A^T A)^{-1}$ we get:
$$\mathbf{x} = (A^T A)^{-1} A^T b$$
The matrix $A^\dagger = (A^T A)^{-1} A^T$ is called **pseudo-inverse** of A.
- If $m < n$ there is a similar "trick".

Summary

- Gaussian elimination algorithm
- Geometrical interpretation of Gaussian elimination operations in 3D
- Gauss-Jordan elimination for inverse calculation
- Inverse calculation algorithm