Lecture 6

Solving Sets of Equations II

Ill-Conditioned Systems, Iterative Methods

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Contents

Solving Sets of Equations

- **The Inverse of a Matrix and Matrix Pathology.** Shows how an important derivative of a matrix, its inverse, can be computed. It shows when a matrix cannot be inverted and tells of situations where no unique solution exists to a system of equations.
- **Ill-Conditioned Systems.** Explores systems for which getting the solution with accuracy is very difficult. A number, the condition number, is a measure of such difficulty. A property of a matrix, called its norm, is used to compute its condition number. A way to improve an inaccurate solution is described.
- **Iterative Methods.** Describes how a linear system can be solved in an entirely different way, by beginning with an initial estimate of the solution and performing computations that eventually arrive at the correct solution. An iterative method is particularly important in solving systems that have few nonzero coefficients.

Using the LU Matrix for Multiple Right-Hand Sides I

- Many physical situations are modelled with a large set of linear equations.
- The equations will depend on the geometry and certain external factors that will determine the right-hand sides.
- If we want the solution for **many different values of these right-hand sides**,
- it is inefficient to solve the system from the start with each one of the right-hand-side values.
- Using the *LU* equivalent of the coefficient matrix is preferred.

Using the LU Matrix for Multiple Right-Hand Sides II

- Suppose we have solved the system $Ax = b$ by Gaussian elimination.
- We now know the LU equivalent of A: $A = L * U$
- Consider now that we want to solve $Ax = b$ with some new b-vector.
- We can write

$$Ax = b$$

$$LUx = b$$

$$Ly = b$$

- The product of U and x is a vector, call it y.
- Now, we can solve for y from $Ly = b$.
- This is readily done because L is lower-triangular and we get y by forward-substitution.
- Call the solution $y = b'$.
- Going back to the original $LUx = b$, we see that, from $Ux = y = b'$, we can get x from $Ux = b'$.
- Which is again readily done by back-substitution (U is upper-triangular).

Using the LU Matrix for Multiple Right-Hand Sides II

- i.e., Solve $Ax = b$, where we already have its L and U matrices:

$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0.66667 & 1 & 0 & 0 \\ 0.33333 & -0.45454 & 1 & 0 \\ 0.0 & -0.54545 & 0.32 & 1 \end{bmatrix} * \begin{bmatrix} 6 & 1 & -6 & -5 \\ 0 & -3.6667 & 4 & 4.3333 \\ 0 & 0 & 6.8182 & 5.6364 \\ 0 & 0 & 0 & 1.5600 \end{bmatrix}$$

- Suppose that the b-vector is $[6\ -7\ -2\ 0]^T$.
- We first get $y = Ux$ from $Ly = b$ by forward substitution:

$$y = [6\ -11\ -9\ -3.12]^T$$

- and use it to compute x from $Ux = y$:

$$x = [-0.5\ 1\ 0.3333\ -2]^T.$$

- Now, if we want the solution with a different b-vector;

$$bb = [1\ 4\ -3\ 1]^T$$

- we just do $Ly = bb$ to get

$$y = [1\ 3.3333\ -1.8182\ 3.4]^T$$

- and then use this y in $Ux = y$ to find the new x:

$$x = [0.0128\ -0.5897\ -2.0684\ 2.1795]^T$$

The Inverse of a Matrix and Matrix Pathology I

- Division by a matrix is not defined but the equivalent is obtained from the *inverse* of the matrix.
- If the product of two square matrices, $A * B$, equals to the *identity matrix*, I, B is said to be the inverse of A (and also A is the inverse of B).
- Matrices do not commute ($A * B \neq B * A$) on multiplication but inverses are an exception: $A * A^{-1} = A^{-1} * A$.
- To find the inverse of matrix A, use an elimination method.
- We augment the A matrix with the identity matrix of the same size and solve. The solution is A^{-1}. Example;

$$A = \begin{bmatrix} 1 & -1 & 2 \\ 3 & 0 & 1 \\ 1 & 0 & 2 \end{bmatrix}, \qquad \begin{bmatrix} 1 & -1 & 2 & 1 & 0 & 0 \\ 3 & 0 & 1 & 0 & 1 & 0 \\ 1 & 0 & 2 & 0 & 0 & 1 \end{bmatrix}, \qquad \begin{matrix} R_2 - (3/1)R_1 \rightarrow \\ R_3 - (1/1)R_1 \rightarrow \end{matrix}$$

$$\begin{bmatrix} 1 & -1 & 2 & 1 & 0 & 0 \\ 0 & 3 & -5 & -3 & 1 & 0 \\ 0 & 1 & 0 & -1 & 0 & 1 \end{bmatrix}, \begin{bmatrix} 1 & -1 & 2 & 1 & 0 & 0 \\ 0 & 1 & 0 & -1 & 0 & 1 \\ 0 & 3 & -5 & -3 & 1 & 0 \end{bmatrix}, \qquad R_3 - (3/1)R_2 \rightarrow$$

The Inverse of a Matrix and Matrix Pathology II

- Cont.

$$\left[\begin{array}{cccccc} 1 & -1 & 2 & 1 & 0 & 0 \\ 0 & 1 & 0 & -1 & 0 & 1 \\ 0 & 0 & -5 & 0 & 1 & -3 \end{array}\right], \quad R_3/(-5) \quad , \quad R_1 - (2/1)R_3 \rightarrow \quad ,$$

$$\left[\begin{array}{cccccc} 1 & -1 & 0 & 1 & 2/5 & -6/5 \\ 0 & 1 & 0 & -1 & 0 & 1 \\ 0 & 0 & 1 & 0 & -1/5 & 3/5 \end{array}\right], \quad R_2 - (1/-1)R_1 \rightarrow \quad ,$$

$$\left[\begin{array}{cccccc} 1 & 0 & 0 & 0 & 2/5 & -1/5 \\ 0 & 1 & 0 & -1 & 0 & 1 \\ 0 & 0 & 1 & 0 & -1/5 & 3/5 \end{array}\right]$$

- We confirm the fact that we have found the inverse by multiplication:

$$\underbrace{\left[\begin{array}{ccc} 1 & -1 & 2 \\ 3 & 0 & 1 \\ 1 & 0 & 2 \end{array}\right]}_{A} * \underbrace{\left[\begin{array}{ccc} 0 & 2/5 & -1/5 \\ -1 & 0 & 1 \\ 0 & -1/5 & 3/5 \end{array}\right]}_{A^{-1}} = \underbrace{\left[\begin{array}{ccc} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{array}\right]}_{I}$$

The Inverse of a Matrix and Matrix Pathology III

- It is more *efficient* to use Gaussian elimination. We show only the final triangular matrix; we used pivoting:

$$\begin{bmatrix} 1 & -1 & 2 & 1 & 0 & 0 \\ 3 & 0 & 1 & 0 & 1 & 0 \\ 1 & 0 & 2 & 0 & 0 & 1 \end{bmatrix} \rightarrow \begin{bmatrix} 3 & 0 & 1 & 0 & 1 & 0 \\ (0.333) & -1 & 1.667 & 1 & -0.333 & 0 \\ (0.333) & (0) & 1.667 & 0 & -0.333 & 1 \end{bmatrix}$$

- After doing the back-substitutions, we get

$$\begin{bmatrix} 3 & 0 & 1 & 0 & 0.4 & -0.2 \\ (0.333) & -1 & 1.667 & -1 & 0 & 1 \\ (0.333) & (0) & 1.667 & 0 & -0.2 & 0.6 \end{bmatrix}$$

- If we have the inverse of a matrix, we can *use it to solve a set of equations*, $Ax = b$,
- because multiplying by A^{-1} gives the answer (x):

$$A^{-1}Ax = A^{-1}b$$
$$x = A^{-1}b$$

Pathological Systems

- When a real physical situation is modelled by a set of linear equations, we can anticipate that the set of equations will have a solution that matches the values of the quantities in the physical problem (**the equations should truly do represent it**).
- Because of round-off errors, the solution vector that is calculated may imperfectly predict the physical quantity, but there is assurance that a solution exists.
- Here is an example of a matrix that has no inverse:

$$A = \begin{bmatrix} 1 & -2 & 3 \\ 2 & 4 & -1 \\ -1 & -14 & 11 \end{bmatrix}$$

```
>> lu(A)
ans =
  2.0000       4.0000      -1.0000
 -0.5000     -12.0000      10.5000
  0.5000       0.3333       0
```

Element A(3,3) cannot be used as a divisor in the back-substitution. That means that **we cannot solve**.

- The definition of a *singular matrix* is a matrix that does not have an inverse.

Redundant Systems I

- Even though a matrix is singular, it may still have a solution. Consider again the same singular matrix:

$$A = \begin{bmatrix} 1 & -2 & 3 \\ 2 & 4 & -1 \\ -1 & -14 & 11 \end{bmatrix}$$

- Suppose we solve the system $Ax = b$ where the right-hand side is $b = [5, 7, 1]^T$.

```
>> Ab=[1 -2 3 5; 2 4 -1 7; -1 -14 11 1]
>> lu (Ab)
ans =
 2.0000       4.0000      -1.0000       7.0000
(-0.5000)   -12.0000      10.5000       4.5000
(0.5000)     (0.3333)      0            0
```

- The back-substitution cannot be done.
  - The output suggests that x_3 can have any value.
  - Suppose we set it equal to 0. We can solve the first two equations with that substitution, that gives $[17/4, -3/8, 0]^T$.
  - Suppose we set x_3 to 1 and repeat. This gives $[3, 1/2, 1]^T$, and this is another solution.
  - We have found a solution, actually, an infinity of them. The reason for this is that the system is **redundant**.

Redundant Systems II

- What we have here is not truly three linear equations but only two independent ones.
- The system is called *redundant*.
- See Table 1 for the comparison of *singular* and *nonsingular* matrices.

Table: A comparison of singular and nonsingular matrices

For Singular matrix A:	For Nonsingular Matrix A:
It has no inverse, A^{-1}	It has an inverse, A^{-1}
Its determinant is zero	The determinant is nonzero
There is no unique solution to the system $Ax = b$	There is a unique solution to the system $Ax = b$
Gaussian elimination cannot avoid a zero on the diagonal	Gaussian elimination does not encounter a zero on the diagonal
The rank is less than n	The rank equals n
Rows are linearly dependent	Rows are linearly independent
Columns are linearly dependent	Columns are linearly independent

Ill-Conditioned Systems I

- A system whose coefficient matrix is singular has **no unique solution**.
- What if the matrix is *almost* singular?

$$A = \begin{bmatrix} 3.02 & -1.05 & 2.53 \\ 4.33 & 0.56 & -1.78 \\ -0.83 & -0.54 & 1.47 \end{bmatrix}$$

- The LU equivalent has a very small element in (3, 3),

$$LU = \begin{bmatrix} 4.33 & 0.56 & -1.78 \\ (0.6975) & -1.4406 & 3.7715 \\ (-0.1917) & (0.3003) & -0.0039 \end{bmatrix},$$

- Inverse has elements very large in comparison to A:

$$inv(A) = \begin{bmatrix} 5.6611 & -7.2732 & -18.5503 \\ 200.5046 & -268.2570 & -66669.9143 \\ 76.8511 & -102.6500 & -255.8846 \end{bmatrix}$$

- Matrix is nonsingular but is *almost* singular.

Ill-Conditioned Systems II

- Suppose we solve the system $Ax = b$, with b equal to $[-1.61, 7.23, -3.38]^T$.
  - The solution is $x = [1.0000, 2.0000, -1.0000]^T$.
- Now suppose that we make a **small change** in just the first element of the b-vector : $[-1.60, 7.23, -3.38]^T$.
  - We get $x = [1.0566, 4.0051, -0.2315]^T$
- if $b = [-1.61, 7.22, -3.38]^T$, the solution now is $x = [1.07271, 4.6826, 0.0265]^T$ which also differs.

```
>> A=[3.02 -1.05 2.53; 4.33 0.56 -1.78; -0.83 -0.54 1.47];
b=[-1.61 7.23 -3.38];A\b'
ans =
    1.0000
    2.0000
   -1.0000
>> A=[3.02 -1.05 2.53; 4.33 0.56 -1.78; -0.83 -0.54 1.47];
b=[-1.60 7.23 -3.38];A\b'
ans =
    1.0566
    4.0050
   -0.2315
>> A=[3.02 -1.05 2.53; 4.33 0.56 -1.78; -0.83 -0.54 1.47];
b=[-1.61 7.22 -3.38];A\b'
ans =
    1.0727
    4.6826
    0.0265
```


Ill-Conditioned Systems III

- A system whose coefficient matrix is nearly singular is called **ill-conditioned**.
- When a system is ill-conditioned, the solution is very sensitive
  - to small changes in the right-hand vector,
  - to small changes in the coefficients.
- $A(1,1)$ is changed from 3.02 to 3.00, original b-vector, a large change in the solution $x = [1.1277, 6.5221, 0.7333]^T$].
- This means that it is also very sensitive to round-off error.

```
>> A=[3.00 -1.05 2.53; 4.33 0.56 -1.78;
      -0.83 -0.54 1.47];
b=[-1.61 7.23 -3.38];A\b'
ans =
    1.1277
    6.5221
    0.7333
```


Norms I

- **Norm**, a measure of the magnitude of the matrix.
- The magnitude of a single number is just its distance from zero:
  $|-4.2| = 4.2$.
- For vectors in two- or three space, norm is called the *Euclidean norm*, and is computed by $\sqrt{x_1^2 + x_2^2 + x_3^2}$.
- We compute the Euclidean norm of vectors with more than three components by

$$||x||_e = \sqrt{x_1^2 + x_2^2 + \ldots + x_n^2} = \left(\sum_{i=1}^{n} x_i^2 \right)^{1/2}$$

- Defining the p-norm as

$$||x||_p = \left(\sum_{i=1}^{n} |x_i|^p \right)^{1/p}$$

Norms II

- Using $||A||$ to represent the norm of matrix A, some properties
  1. $||A|| \geq 0$ and $||A|| = 0$ if and only if $A = 0$
  2. $||kA|| = ||k||||A||$
  3. $||A + B|| \leq ||A|| + ||B||$
  4. $||AB|| \leq ||A||||B||$
- 1-, 2-, and ∞-norms;

$$||x||_1 = \sum_{i=1}^{n} |x_i| = \textit{sum of magnitudes}$$
$$||x||_2 = \left(\sum_{i=1}^{n} |x_i|^2\right)^{1/2} = \textit{Euclidean norm}$$
$$||x||_\infty = max_{1 \leq i \leq n} |x_i| = \textit{maximum} - \textit{magnitude norm}$$

- i.e., Compute the 1-, 2-, and ∞-norms of the vector $x = (1.25, 0.02, -5.15, 0)$

$$||x||_1 = |1.25| + |0.02| + |-5.15| + |0| = 6.42$$
$$||x||_2 = 5.2996$$
$$||x||_\infty = 5.15$$

Matrix Norms I

- The norms of a matrix are similar to the norms of a vector.

$$||A||_1 = max_{1 \le j \le n} \sum_{i=1}^{n} |a_{ij}| = \textit{maximum column sum}$$
$$||A||_\infty = max_{1 \le i \le n} \sum_{j=1}^{n} |a_{ij}| = \textit{maximum row sum}$$

- For an $m \times n$ matrix, the Frobenius norm is defined as

$$||A||_f = \left(\sum_{i=1}^{m} \sum_{j=1}^{n} a_{ij}^2 \right)^{1/2}$$

  The Frobenius norm is a good measure of the magnitude of a matrix.
- Suppose r is the largest eigenvalue of $A^T * A$. Then $||A||_2 = r^{1/2}$.
- This is called the *spectral norm* of A, and $||A||_2$ is always less than (or equal to) $||A||_1$ and $||A||_\infty$.
- The spectral norm is usually the most *expensive*.
- Which norm is best? In most instances, we want the norm that puts the smallest upper bound on the magnitude of the matrix.
- In this sense, the spectral norm is usually the ”best”.

Matrix Norms II

```
A =
  5 -5 -7
 -4  2 -4
 -7 -4  5
>> norm(A,'fro')
ans =
15
>> norm(A,inf)
ans =
17
>> norm(A,1)
ans=
16
>> norm(A)
ans =
12.0301
>> norm (A,2)
ans =
12.0301
```

we observe that the 2-norm, the spectral norm, is the norm we get if we just ask for the norm. The smallest norm of the matrix is the spectral norm, it is the tightest measure.

Iterative Methods I

- Gaussian elimination and its variants are called ***direct methods***.
- An entirely different way to solve many systems is through ***iteration***.
- In this way, we start with an initial estimate of the solution vector and proceed to refine this estimate.
- The two methods for solving $Ax = b$ are
  1. the *Jacobi Method* ,
  2. the *Gauss-Seidel Method*.

Iterative Methods II

- An $n \times n$ matrix A is *diagonally dominant* if and only if;

$$|a_{ii}| > \sum_{j=1, j \neq i}^{n} |a_{ij}|, i = 1, 2, \ldots, n$$

- Although this may seem like a very restrictive condition, it turns out that there are very many applied problems that have this property.
- i.e.,

$$\begin{aligned} 6x_1 - 2x_2 + x_3 &= 11 \\ x_1 + 2x_2 - 5x_3 &= -1 \\ -2x_1 + 7x_2 + 2x_3 &= 5 \end{aligned}$$

- The solution is $x_1 = 2, x_2 = 1, x_3 = 1$.
- However, before we begin our iterative scheme we must first reorder the equations so that the coefficient matrix is diagonally dominant.

Jacobi Method I

- After reordering;

$$\begin{aligned} 6x_1 - 2x_2 + x_3 &= 11 \\ -2x_1 + 7x_2 + 2x_3 &= 5 \\ x_1 + 2x_2 - 5x_3 &= -1 \end{aligned}$$

  Is the solution same? Check it out as an exercise.
- The iterative methods depend on the rearrangement of the equations in this manner:

$$x_i = \frac{b_i}{a_{ii}} - \sum_{j=1, j\neq i}^{n} \frac{a_{ij}}{a_{ii}} x_j, i = 1, 2, \ldots, n, \mapsto x_1 = \frac{11}{6} - \left(\frac{-2}{6} x_2 + \frac{1}{6} x_3 \right)$$

- Each equation now solved for the variables in succession:

$$\begin{aligned} x_1 &= 1.8333 + 0.3333x_2 - 0.1667x_3 \\ x_2 &= 0.7143 + 0.2857x_1 - 0.2857x_3 \\ x_3 &= 0.2000 + 0.2000x_1 + 0.4000x_2 \end{aligned} \quad (1)$$

- We begin with some initial approximation to the value of the variables.
- Say initial values are; $x_1 = 0, x_2 = 0, x_3 = 0$.
- Each component might be taken equal to *zero if no better initial estimates* are at hand.

Jacobi Method II

- Note that this method is exactly the same as the method of fixed-point iteration for a single equation that was discussed in Section **??**.
- But it is now applied to a set of equations; we see this if we write Eqn. 1 in the form of

$$x^{(n+1)} = G(x^{(n)}) = b' - Bx^n$$

  which is identical to $x_{n+1} = g(x_n)$ as used in Section **??**.
- The new values are substituted in the right-hand sides to generate a second approximation,
- and the process is repeated until successive values of each of the variables are sufficiently alike.
- Now, general form

$$\begin{aligned} x_1^{(n+1)} &= 1.8333 + 0.3333x_2^{(n)} - 0.1667x_3^{(n)} \\ x_2^{(n+1)} &= 0.7143 + 0.2857x_1^{(n)} - 0.2857x_3^{(n)} \\ x_3^{(n+1)} &= 0.2000 + 0.2000x_1^{(n)} + 0.4000x_2^{(n)} \end{aligned} \qquad (2)$$

Jacobi Method III

- Starting with an initial vector of $x^{(0)} = (0, 0, 0,)$, we obtain Table 2

	First	Second	Third	Fourth	Fifth	Sixth	...	Ninth
x_1	0	1.833	2.038	2.085	2.004	1.994	...	2.000
x_2	0	0.714	1.181	1.053	1.001	0.990	...	1.000
x_3	0	0.200	0.852	1.080	1.038	1.001	...	1.000

Table: Successive estimates of solution (Jacobi method)

- In the present context, $x^{(n)}$ and $x^{(n+1)}$ refer to the n^{th} and $(n+1)^{st}$ iterates of a vector rather than a simple variable, and g is a linear transformation rather than a nonlinear function.
- Rewrite in matrix notation; let $A = L + D + U$,

$$Ax = b, \begin{bmatrix} 6 & -2 & 1 \\ -2 & 7 & 2 \\ 1 & 2 & -5 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 11 \\ 5 \\ -1 \end{bmatrix}$$

$$L = \begin{bmatrix} 0 & 0 & 0 \\ -2 & 0 & 0 \\ 1 & 2 & 0 \end{bmatrix}, D = \begin{bmatrix} 6 & 0 & 0 \\ 0 & 7 & 0 \\ 0 & 0 & -5 \end{bmatrix}, U = \begin{bmatrix} 0 & -2 & 1 \\ 0 & 0 & 2 \\ 0 & 0 & 0 \end{bmatrix}$$

Jacobi Method IV

$$Ax = (L + D + U)x = b$$
$$Dx = -(L + U)x + b$$
$$x = -D^{-1}(L + U)x + D^{-1}b$$

- From this we have, identifying x on the left as the new iterate,

$$x^{(n+1)} = -D^{-1}(L + U)x^{(n)} + D^{-1}b$$

In Eqn. 2,

$$b' = D^{-1}b = \begin{bmatrix} 1.8333 \\ 0.7143 \\ 0.2000 \end{bmatrix}$$

$$D^{-1}(L + U) = \begin{bmatrix} 0 & -0.3333 & 0.1667 \\ -0.2857 & 0 & 0.2857 \\ -0.2000 & -0.4000 & 0 \end{bmatrix}$$

- This procedure is known as the Jacobi method, also called "*the method of simultaneous displacements*",
- because each of the equations is simultaneously changed by using the most recent set of x-values (see Table 2).

Gauss-Seidel Iteration I

- Even though we have $newx^1$ available, we do not use it to compute $newx^2$.
- In nearly all cases the new values are better than the old and ought to be used instead.
- When this done, the procedure known as *Gauss-Seidel* iteration.
- We proceed to improve each x-value in turn, using always the most recent approximations of the other variables.

	First	Second	Third	Fourth	Fifth	Sixth
x_1	0	1.833	2.069	1.998	1.999	2.000
x_2	0	1.238	1.002	0.995	1.000	1.000
x_3	0	1.062	1.015	0.998	1.000	1.000

Table: Successive estimates of solution (Gauss-Seidel method)

Gauss-Seidel Iteration II

- These values were computed by using this iterative scheme:

$$
\begin{aligned}
x_1^{(n+1)} &= 1.8333 + 0.3333x_2^{(n)} - 0.1667x_3^{(n)} \\
x_2^{(n+1)} &= 0.7143 + 0.2857x_1^{(n+1)} - 0.2857x_3^{(n)} \\
x_3^{(n+1)} &= 0.2000 + 0.2000x_1^{(n+1)} + 0.4000x_2^{(n+1)}
\end{aligned}
$$

  beginning with $x^{(1)} = (0, 0, 0)^T$

- The rate of convergence is more rapid than for the Jacobi method (see Table 3).