NENG 685, Class 5, Fall 2017

Vectors, Matrices, and Systems of Equations: October 18, 2017

Note: Course notes 05-01 contains a more thorough review of linear algebra concepts. This here is very high level with the intention of moving quickly to solving these systems numerically.

Vector Review

A real n-dimensional vector $\vec{x}$ is an ordered set of n real numbers that expresses magnitude and direction:

$$\vec{x} = (x_1, x_2, \dots, x_n)$$

Properties:

1. sum: two vectors of the same size give a new vector of that size: $\vec{x} + \vec{y} = (x_1 + y_1, x_2 + y_2, \dots, x_n + y_n)$
2. scalar multiple: $c\vec{x} = (cx_1, cx_2, \dots, cx_n)$
3. dot product: takes two equal length vectors and results in a scalar.

   Algebraically, it is the sum of the products of the corresponding entries of the two sequences of numbers: $\vec{x} \cdot \vec{y} = \sum_{i=1}^{n} a_i b_i = x_1 y_1 + x_2 y_2 + \cdots + x_n y_n$

   Geometrically, it is the product of the magnitudes of the two vectors and the cosine of the angle between them. $\vec{x} \cdot \vec{y} = ||\vec{x}|| ||\vec{y}|| cos\theta$.
4. $||\vec{x}||^2 = \vec{x} \cdot \vec{x}$
5. distance from $\vec{x}$ to $\vec{y}$: $||\vec{x} - \vec{y}|| = ((x_1 - y_1)^2 + (x_2 - y_2)^2 + \cdots + (x_n - y_n)^2)^{1/2}$
6. commutative property: $\vec{x} + \vec{y} = \vec{y} + \vec{x}$
7. associative property: $(\vec{x} + \vec{y}) + \vec{z} = \vec{x} + (\vec{y} + \vec{z})$
8. distributive property: $c(\vec{x} + \vec{y}) = c\vec{x} + c\vec{y}$

Matrix Review

$$\mathbf{A} = [a_{ij}]_{m\times n} = \begin{pmatrix} a_{11} & a_{12} & \cdots & a_{1j} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2j} & \cdots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots & \ddots & \vdots \\ a_{i1} & a_{i2} & \cdots & a_{ij} & \cdots & a_{in} \\ \vdots & \vdots & \ddots & \vdots & \ddots & \vdots \\ a_{m1} & a_{m2} & \cdots & a_{mj} & \cdots & a_{mn} \end{pmatrix}$$

where $i = 1, \ldots, m$ is the row index and $j = 1, \ldots, n$ is the column index.

$\mathbf{A} \in \mathbb{R}^{m\times n}$ is an $m \times n$ real matrix
$\mathbf{A} \in \mathbb{C}^{m\times n}$ is an $m \times n$ complex matrix

Properties

1. sum: $\mathbf{A} + \mathbf{B} = [a_{ij} + b_{ij}]_{m\times n}$
2. scalar multiple: $c\mathbf{A} = [ca_{ij}]_{m\times n}$
3. multiplication: $\mathbf{C} = \mathbf{AB}$;

   $\mathbf{A} \in \mathbb{C}^{m\times n}$, and $\mathbf{B} \in \mathbb{C}^{n\times p}$, and $\mathbf{C} \in \mathbb{C}^{m\times p}$, then $c_{ij} = \sum_{k=1}^{n} a_{ik}b_{kj}$

   $\mathbf{AB} \neq \mathbf{BA}$
4. commutative property: $\mathbf{A} + \mathbf{B} = \mathbf{B} + \mathbf{A}$
5. associative property: $(\mathbf{A} + \mathbf{B}) + \mathbf{C} = \mathbf{A} + (\mathbf{B} + \mathbf{C})$
6. distributive property: $c(\mathbf{A} + \mathbf{B}) = c\mathbf{A} + c\mathbf{B}$

Definitions

Given $\mathbf{A} \in \mathbb{C}^{m\times n}$, $\mathbf{A}$ is

1. Transpose: $\mathbf{A} \in \mathbb{C}^{m\times n}$, and $\mathbf{B} \in \mathbb{C}^{n\times m} = \mathbf{A}^T$ from

$b_{ij} = a_{ji}$ for $i = 1, \ldots, n$ and $j = 1, \ldots, m$

$$\mathbf{A} = \begin{pmatrix} 1-i & 2 \\ 3+2i & 4 \\ 5 & 6+0.4i \end{pmatrix}, \qquad \mathbf{A}^T = \begin{pmatrix} 1-i & 3+2i & 5 \\ 2 & 4 & 6+0.4i \end{pmatrix}$$

2. Inverse: $\mathbf{A}\mathbf{A}^{-1} = \mathbf{A}^{-1}\mathbf{A} = \mathbf{I}$, where $\mathbf{I}$ is a diagonal matrix containing ones on the diagonal. If this exists, $\mathbf{A}$ is non-singular / invertible.

$$\mathbf{A} = \begin{pmatrix} 4 & 3 \\ 3 & 2 \end{pmatrix}$$

$$\mathbf{A}^{-1} = \begin{pmatrix} -2 & 3 \\ 3 & -4 \end{pmatrix}$$

3. Symmetric if $\mathbf{A} = \mathbf{A}^T$

$$\mathbf{A} = \mathbf{A}^T = \begin{pmatrix} 1 & 2 \\ 2 & 3 \end{pmatrix}$$

4. Orthogonal if A is real and $\mathbf{A}\mathbf{A}^T = \mathbf{A}^T\mathbf{A}$, which means $\mathbf{A}^{-1} = \mathbf{A}^T$.

$$\mathbf{A} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}, \qquad \mathbf{A}^T = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}, \qquad \mathbf{A}^T\mathbf{A} = \frac{1}{2}\begin{pmatrix} 2 & 0 \\ 0 & 2 \end{pmatrix} = \mathbf{I}$$

Equations and Special Matrices

All of the information above is context to help us solve actual problems.

We often write systems of equations as $\mathbf{A}\vec{x} = \vec{b}$ from

$$\begin{aligned} &a_{11}x_1 + a_{12}x_2 + \cdots + a_{1n}x_n = b_1 \\ &\vdots \\ &a_{n1}x_1 + a_{n2}x_2 + \cdots + a_{nn}x_n = b_n \end{aligned}$$

To find $\vec{x}$, we need to find a way to affect $\mathbf{A}^{-1}\vec{b}$. This can be done many many ways, and the first thing we'll talk about are methods for inverting the matrix.

- Tridiagonal matrix has entries on only the main, upper, and lower diagonal
- Lower triangular has entries on the diagonal and below
- Upper triangular has entries on the diagonal and above
- Block Tridagonal has blocks of elements (like sub-matrices) on the diagonal. The blocks may be full or only partially full. The blocks look like $\mathbf{D}_k = [\mathbf{D_{ij}}]_k$

The inverse of a diagonal is simply: $d_{ii}^{-1} = 1/d_{ii}$, another diagonal matrix.

Theorem: The following are equivalent (see Math 54 or a textbook for proof):

1. $\mathbf{A}$ is regular ($\mathbf{A}^{-1}$ exists)
2. Rank($\mathbf{A}$) = n
3. $\mathbf{A}\vec{x} = 0$ if $x = 0$
4. $\mathbf{A}\vec{x} = \vec{b}$ is uniquely solvable $\forall\vec{b}$
5. det($\mathbf{A}$) $\neq 0$

Minors, Cofactors, Determinants

If the determinant is zero, then the matrix is singular, meaning we cannot invert it and numerical solutions are pretty much impossible.

Properties of Determinants

- det($\alpha\mathbf{A}$) = α^n det($\mathbf{A}$)
- det($\mathbf{A}^T$) = det($\mathbf{A}$)
- det($\mathbf{A}^{-1}$) = 1/det($\mathbf{A}$)
- det($\mathbf{AB}$) = det($\mathbf{A}$)det($\mathbf{B}$)
- det($\mathbf{A}^k$) = [det($\mathbf{A}$)]^k
- in general, det($\mathbf{A} + \mathbf{B}$) $\neq$ det($\mathbf{A}$) + det($\mathbf{B}$)

Good illustration: http://www.mathsisfun.com/algebra/matrix-inverse-minors-cofactors-adjugate.html

For a square matrix, the **first order minor**, M_{ij}, just deletes the i^{th} row and j^{th} column and takes the determinant. E.g.

$$\mathbf{A} = \begin{pmatrix} 1 & 4 & 7 \\ 3 & 0 & 5 \\ -1 & 9 & 11 \end{pmatrix} \qquad M_{23} = \det \begin{pmatrix} 1 & 4 \\ -1 & 9 \end{pmatrix} = ((1 \times 9) - (4 \times -1)) = 13$$

The corresponding i, j **cofactor** of $\mathbf{A}$ is

$$C_{ij} = (-1)^{i+j} M_{ij}$$

You can compute minors and cofactors for all of $\mathbf{A}$. The $n \times n$ matrix containing all of the cofactors is denoted $\mathbf{C}$ in this context.

Using these terms, the <u>determinant</u> (which we use for lots of stuff) can be defined in terms of the Laplace expansion

$$\begin{aligned} \det(\mathbf{A}) &= \sum_{j=1}^{n} a_{ij} C_{ij} \text{ for any i} \in \{1, ..., n\} \\ &= \sum_{i=1}^{n} a_{ij} C_{ij} \text{ for any j} \in \{1, ..., n\} \end{aligned}$$

For the above matrix, lets look at the Laplace expansion along the second column ($j = 2$; sum runs over i)

$$\begin{aligned} \det(\mathbf{A}) &= (-1)^{1+2} a_{12} M_{12} + (-1)^{2+2} a_{22} M_{22} + (-1)^{3+2} a_{32} M_{32} \\ &= (-1)^{1+2} \cdot 4 \cdot \det \begin{pmatrix} 3 & 5 \\ -1 & 11 \end{pmatrix} + (-1)^{2+2} \cdot 0 \cdot \det \begin{pmatrix} 1 & 7 \\ -1 & 11 \end{pmatrix} + (-1)^{3+2} \cdot 9 \cdot \det \begin{pmatrix} 1 & 7 \\ 3 & 5 \end{pmatrix} \\ &= -4 \cdot ((3 \cdot 11) - (5 \cdot -1)) + 0 - 9 \cdot ((1 \cdot 5) - (7 \cdot 3)) = -8 \end{aligned}$$

The inverse of $\mathbf{A}$ (which we often need) can be obtained from the determinant and cofactor matrix:

$$\mathbf{A}^{-1} = \frac{1}{\det(\mathbf{A})} \mathbf{C}^T$$

The benefit is that if we've used the cofactor method to get the determinant then we get the inverse for free.

We'll explore this concept in the 05-3 ipython notebook section of this lecture.

Norms and Convergence

We're going to look at direct and iterative methods to solve problems; we'll need these concepts to understand how the solution methods behave.

Vector Norms

A norm is a function that assigns a strictly positive length or size to each vector in a vector space.

Given $\vec{x}, \vec{y} \in \mathbb{R}^n$, a vector norm, denoted by $|| \cdot ||$, has the following properties:

1. $||\vec{x}|| > 0$; $||\vec{x}|| = 0$ iff $\vec{x} = 0$ (positive definite)
2. $||\vec{x} + \vec{y}|| \leq ||\vec{x}|| + ||\vec{y}||$ (triangle inequality)
3. $||\alpha\vec{x}|| = |\alpha| \; ||\vec{x}||$ (homogeneous)

The p-norm:

$$||\vec{x}||_p \equiv (|x_1|^p + |x_2|^p + \cdots + |x_n|^p)^{1/p} \qquad p \geq 1$$

- $||\vec{x}||_1 \equiv |x_1| + |x_2| + \cdots + |x_n|$
- Euclidean norm (length) $||\vec{x}||_2 \equiv (|x_1|^2 + |x_2|^2 + \cdots + |x_n|^2)^{1/2}$
- $||\vec{x}||_\infty \equiv \max\limits_{1 \leq i \leq n} |x_i|$

Convergence

We can use the concepts of norms and inner products to develop some relationships and talk about convergence. Note that there are two ways we think of convergence in numerical methods:

1. the **method**: the speed at which a numerical guess approaches the true solution with iteration count;
2. the **discretization**: speed at which a numerical guess approaches the true solution with reduction in grid size.

In numerical analysis, the speed at which a convergent sequence approaches its limit is what is commonly called the *rate of convergence*. This concept is of practical importance in dealing with a sequence of successive approximations for an iterative method, as then typically fewer iterations are needed to yield a useful approximation if the rate of convergence is higher.

We will first talk about this and we will use the *Cauchy-Schwartz* inequality:

$$\langle \vec{x}, \vec{y} \rangle \leq ||\vec{x}||_2 ||\vec{y}||_2$$

Two norms, denoted $||\cdot||_a$ and $||\cdot||_b$ here, are defined as being equivalent if there exists C_1 and C_2 such that $\forall \vec{x} \in \mathbb{R}^n$

$$C_1||\vec{x}||_a \leq ||\vec{x}||_b \leq C_2||\vec{x}||_a \qquad \text{where } C_1, C_2 = f(n)$$

This leads to the theorem that in $\mathbb{R}^n$ all norms are equivalent (offered without proof). E.g.:

$$\begin{aligned} ||\vec{x}||_\infty &\leq ||\vec{x}||_2 \leq \sqrt{n}||\vec{x}||_\infty \\ ||\vec{x}||_\infty &\leq ||\vec{x}||_1 \leq n||\vec{x}||_\infty \\ ||\vec{x}||_2 &\leq ||\vec{x}||_1 \leq \sqrt{n}||\vec{x}||_2 \end{aligned}$$

The inequalities above may not be ‘sharp’ (A sharp inequality is when there could be no better inequality when making the comparison).

E.g., when comparing two real numbers/expressions, an inequality is sharp because we could not increase the left or decrease the right by a positive factor and still have it be true ($2 \leq 2$).

Norm equivalence is very important because if we can prove some property (usually convergence or an error bound) in **some** norm, we have effectively proven it in **all** norms.

Error

For $\vec{x}$ (the real solution) and $\hat{x}$ (representing our numerical solution) $\in \mathbb{R}^n$ and some norm p we define

- Absolute error: $||\hat{x} - \vec{x}||_p$
- Relative error: $\dfrac{||\hat{x} - \vec{x}||_p}{||\vec{x}||_p}$, where $\vec{x} \neq 0$

Convergence

Given a sequence $\{\hat{x}^{(k)}\}_{k=1,2,\ldots,\infty}$ and some norm p, we say that $\{\hat{x}^{(k)}\}$ converges to $\vec{x}$ if

$$\lim_{k\to\infty} ||\hat{x}^{(k)} - \vec{x}||_p = 0$$

When we think of the **rate of convergence**, we can look at how quickly this limit is reached. We measure this as

$$\lim_{k\to\infty} \frac{||\hat{x}^{(k+1)} - \vec{x}||_p}{||\hat{x}^{(k)} - \vec{x}||_p^q} = \mu$$

Here $q \geq 1$ is called the *order of convergence* and μ is the *rate of convergences*. Also written as

$$||\hat{x}^{(k+1)} - \vec{x}||_p = \mu||\hat{x}^{(k)} - \vec{x}||_p^q \to ||e_{k+1}||_p = \mu||e_k||_p^q\,.$$

Consider

- If $q = 1$ and μ varies with iteration ($\mu = \mu_k$), $||e_{k+1}||_p = \mu_k||e_k||_p < ||e_k||_p$, then
  - if $\mu_k \to 1$ as $k \to \infty$, the convergence is sublinear
  - if $\mu_k \to 0$ as $k \to \infty$, the convergence is superlinear
- If $q = 2$, $||e_{k+1}||_p = \mu||e_k||_p^2, \quad (\mu > 0)$, the convergence is quadratic.
- If $q = 3$, $||e_{k+1}||_p = \mu||e_k||_p^3, \quad (\mu > 0)$, the convergence is cubic.

Similar concepts are used for **discretization methods**. The solution of the discretized problem converges to the solution of the continuous problem as the grid size goes to zero, and the speed of convergence is one of the factors of the efficiency of the method. The important parameter here for the convergence speed is not the iteration number k but it depends on the number of grid points and grid spacing. In this case, the number of grid points n in a discretization process is inversely proportional to the grid spacing.

We talked about this during integration.

In this case, a sequence x_n is said to converge to L with order p if there exists a constant C such that

$$\|x_n - L\| < Cn^{-p} \quad \forall\, n\ .$$

This is written as $\|xn - L\| = O(np)$ using the "big O" notation.

This is the relevant definition when discussing methods for numerical quadrature or the solution of ordinary differential equations. A practical method to calculate the rate of convergence for a discretization method is to implement the following formula:

$$p \approx \frac{\log \frac{e_{new}}{e_{old}}}{\log \frac{h_{new}}{h_{old}}}$$

Matrix Norms

Given $\mathbf{A}, \mathbf{B} \in \mathbb{R}^{m\times n}$, a matrix norm, denoted by $||\cdot||$, has the following properties:

1. $||\mathbf{A}|| > 0$ and $||\mathbf{A}|| = 0$ iff $\mathbf{A} = 0$ (positive definite)
2. $||\mathbf{A} + \mathbf{B}|| \leq ||\mathbf{A}|| + ||\mathbf{B}||$ (triangle inequality)
3. $||\alpha\mathbf{A}|| = |\alpha|\ ||\mathbf{A}||$ (homogeneous)

E.g., the Frobenius norm

$$||\mathbf{A}||_F = \sqrt{\sum_{i=1}^{m}\sum_{j=1}^{n} |a_{ij}|^2}$$

Definitions:

- submultiplicative if $||\mathbf{AB}|| \leq ||\mathbf{A}||\ ||\mathbf{B}||$
- Not all norms are submultiplicative; *we will only deal with those that are.*
- subordinate matrix norm for $\mathbf{A} \in \mathbb{R}^{m\times n}$ and $\vec{x} \in \mathbb{R}^n$:
  $||\mathbf{A}|| \equiv \sup\limits_{\vec{x}\neq\vec{0}} \dfrac{||\mathbf{A}\vec{x}||}{||\vec{x}||}$

- **supremum**, or least upper bound, of a set S of real numbers is denoted by sup$S$ and is defined to be the smallest real number that is greater than or equal to every number in S.

  Consequently, the supremum is also referred to as the least upper bound (or LUB). If the supremum exists, it is unique, meaning that there will be only one supremum.

examples:

$$||\mathbf{A}||_1 = \sup_{\vec{x}\neq\vec{0}} \frac{||\mathbf{A}\vec{x}||_1}{||\vec{x}||_1} = \max_{1\leq j\leq n} \sum_{i=1}^{m} |a_{ij}| \qquad \text{max absolute col sum}$$

$$||\mathbf{A}||_\infty = \sup_{\vec{x}\neq\vec{0}} \frac{||\mathbf{A}\vec{x}||_\infty}{||\vec{x}||_\infty} = \max_{1\leq i\leq m} \sum_{j=1}^{n} |a_{ij}| \qquad \text{max absolute row sum}$$

$$||\mathbf{A}||_2 = \sup_{\vec{x}\neq\vec{0}} \frac{||\mathbf{A}\vec{x}||_2}{||\vec{x}||_2} = \text{ the sqrt of the max eigenvalue of } \mathbf{A}^H\mathbf{A}$$

is largest singular value for any matrix, or the spectral radius of a square matrix

For vectors, the infinity norm is the largest value. For matrices, it's the maximum absolute row sum—which is really the row that will most strongly change a vector, so that's analogous. For the 1 matrix norm, the maximum absolute column sum corresponds to the vector component that will, overall, be changed the most. We'll talk about the 2 matrix norm after we talk about spectral radius, which will require a quick review of eigenvalues.

The equivalence of norms we talked about with vectors also holds here. Some of the relationships are

$$||\mathbf{A}||_2 \leq ||\mathbf{A}||_F \leq \sqrt{n}||\mathbf{A}||_2$$
$$\frac{1}{\sqrt{n}}||\mathbf{A}||_\infty \leq ||\mathbf{A}||_2 \leq \sqrt{m}||\mathbf{A}||_\infty$$
$$\frac{1}{\sqrt{m}}||\mathbf{A}||_1 \leq ||\mathbf{A}||_2 \leq \sqrt{n}||\mathbf{A}||_2$$

Again, as with vector norms, showing a property in some matrix norms implies that property in other matrix norms (which may be harder to compute). The inequalities above may not be 'sharp'.

Eigenvalue Review

Eigenvalues are a special set of scalars associated with a linear system of equations (a matrix equation) that are sometimes also known as characteristic roots.

Each eigenvalue is paired with a corresponding so-called eigenvector (or, in general, a corresponding right eigenvector and a corresponding left eigenvector; there is no analogous distinction between left and right for eigenvalues).

The decomposition of a square matrix $\mathbf{A}$ into eigenvalues and eigenvectors is known as eigen decomposition, and the fact that **this decomposition is always possible as long as the matrix consisting of the eigenvectors of $\mathbf{A}$ is square** is known as the eigen decomposition theorem.

Let $\mathbf{A} \in \mathbb{R}^{n \times n}$. If there is a vector $\vec{x} \in \mathbb{R}^n$ such that

$$\mathbf{A}\vec{x} = \lambda\vec{x}$$

for some scalar λ, then λ is an eigenvalue of $\mathbf{A}$ with a corresponding (right) eigenvector $\vec{x}$. Note that the eigenvalue represents the "stretching factor" in the direction of its associated eigenvector.

(http://math.stackexchange.com/questions/54176/is-there-a-geometric-meaning-of-the-frobenius-norm)

We find eigenvalues by re-writing the stated relationship as $(\mathbf{A} - \lambda\mathbf{I})\vec{x} = 0$ and solving for the λs that make this true. The λs are then the eigenvalues and the $\vec{x}$s that go with them are the corresponding eigenvectors.

A linear system of equations has nontrivial solutions if the determinant vanishes (Cramer's rule; related to the theorem for finding out if a solution exits that we talked about above), so the solutions of this equation are given by

$$\det(\mathbf{A} - \lambda\mathbf{I}) = 0 \, .$$

This equation is known as the characteristic equation of $\mathbf{A}$, and the left-hand side is known as the characteristic polynomial.

Example

$$\mathbf{A} = \begin{pmatrix} 2 & 3 \\ 3 & -6 \end{pmatrix} \qquad \mathbf{A} - \lambda\mathbf{I} = \begin{pmatrix} 2-\lambda & 3 \\ 3 & -6-\lambda \end{pmatrix}$$

$$\begin{aligned} \det(\mathbf{A} - \lambda\vec{I}) &= (2-\lambda)(-6-\lambda) - (3)(3) \\ &= -12 + 6\lambda - 2\lambda + \lambda^2 - 9 \\ &= \lambda^2 + 4\lambda - 21 = 0 \\ 0 &= (\lambda - 3)(\lambda + 7) \\ &\boxed{\lambda = 3, -7} \end{aligned}$$

- Eigenvalues may be real or complex.
- Since an n^{th} degree polynomial has n roots, $\mathbf{A}_{n\times n}$ is guaranteed to have n real and/or complex eigenvalues, some of which may be repeated: $\lambda_1, \lambda_2, \ldots, \lambda_n$.

  This gives $\mathbf{A}\vec{u}_1 = \lambda_1\vec{u}_1$, etc.
- Left eigenvectors are found by reformulating the equation as $\vec{y}\mathbf{A} = \alpha\vec{y}$. In nuclear, we're used to seeing the right eigenvector formulation.

The spectrum of eigenvalues of a matrix $\mathbf{A}$ are defined formally as

$$\sigma(\mathbf{A}) = [\lambda \in \mathbb{C} : \det(\mathbf{A} - \lambda\mathbf{I}) = 0]$$

and an eigenvalue is

$$\lambda \in \sigma(\mathbf{A})\ ,$$

and

- $\sigma(\mathbf{A}) = \sigma(\mathbf{A}^T)$
- $\overline{\sigma(\mathbf{A})} = \sigma(\mathbf{A}^H)$