# Appendix 1

# Analysis and Differential Equations

In this appendix we review briefly and without proofs some of the basic results from calculus and ordinary differential equations that are used in the text.

MEAN-VALUE THEOREM: *If the function $f$ is continuously differentiable on an interval $[a, b]$, then there is a point $\xi$ between $a$ and $b$ such that*

$$f(b) - f(a) = f'(\xi)(b - a). \tag{A.1.1}$$

TAYLOR EXPANSION: *If the function $f$ is $k$ times continuously differentiable on an interval $[a, b]$, then for any $x$ and $x_0$ between $a$ and $b$, there is a $\xi$ between $x$ and $x_0$ such that*

$$\begin{aligned} f(x) = {} & f(x_0) + f'(x_0)(x - x_0) + \tfrac{1}{2} f''(x_0)(x - x_0)^2 + \cdots \\ & + \frac{1}{(k-1)!} f^{(k-1)}(x_0)(x - x_0)^{(k-1)} + \frac{1}{k!} f^{(k)}(\xi)(x - x_0)^k. \end{aligned} \tag{A.1.2}$$

Note that the mean-value theorem can be considered a special case of the Taylor expansion for $k = 1$ and $a = x_0$, $b = x$.

CHAIN RULE: *If $f$ and $g$ are two differentiable functions, then the composite function $h(x) = f(g(x))$ is differentiable, and*

$$h'(x) = f'(g(x))g'(x). \tag{A.1.3}$$

SECOND MEAN-VALUE THEOREM OF THE INTEGRAL CALCULUS: *If $u$ and $v$ are continuous functions on the interval $[a,b]$ and $v$ does not change sign in $[a,b]$, then there is a $\xi \in [a,b]$ such that*

$$\int_a^b u(x)v(x)dx = u(\xi)\int_a^b v(x)dx. \tag{A.1.4}$$

The next results deal with functions of several variables $f(x_1,\ldots,x_n)$, or $f(\mathbf{x})$ where $\mathbf{x}$ is the vector with components $x_1,\ldots,x_n$. The partial derivative of $f$ with respect to the $i$th variable is defined at a point $\mathbf{x}$ by

$$\frac{\partial f}{\partial x_i}(\mathbf{x}) = \lim_{h\to 0}\frac{1}{h}[f(x_1,\ldots,x_{i-1},x_i+h,x_{i+1},\ldots,x_n) - f(\mathbf{x})], \tag{A.1.5}$$

and similarly for partial derivatives of higher order. The *derivative* of $f$ at a point $\mathbf{x}$ is defined by

$$f'(\mathbf{x}) = \left(\frac{\partial f}{\partial x_1}(\mathbf{x}),\ldots,\frac{\partial f}{\partial x_n}(\mathbf{x})\right), \tag{A.1.6}$$

and is considered to be a row vector. The transpose of this vector is sometimes called the *gradient* of $f$ and is denoted by $\nabla f$. In this context, it is often convenient to view $\nabla$ as the vector operator of partial derivatives:

$$\nabla = \left(\frac{\partial}{\partial x_1},\ldots,\frac{\partial}{\partial x_n}\right).$$

Then, the operator $\nabla^2$, often denoted by $\Delta$, is the dot product of $\nabla$ with itself, so that

$$\Delta f = \nabla^2 f = \frac{\partial^2 f}{\partial x_1^2} + \cdots + \frac{\partial^2 f}{\partial x_n^2}.$$

This sum of second partial derivatives is very important in the study of partial differential equations (see Chapters 8 and 9).

The function $f$ is said to be continuously differentiable in some region of $n$ space if each (first) partial derivative of $f$ exists and is continuous within that region. For functions of several variables the mean-value theorem again holds, as follows.

MEAN-VALUE THEOREM FOR FUNCTIONS OF SEVERAL VARIABLES: *If $f$ is a continuously differentiable function of $n$ variables in some region, and if $\mathbf{x}$ and $\mathbf{y}$ are two points such that the points*

$$t\mathbf{x} + (1-t)\mathbf{y}, \qquad 0 \le t \le 1$$

*are all in the region, then there is a $\xi$ between 0 and 1 such that*

$$f(\mathbf{y}) - f(\mathbf{x}) = f'(\xi\mathbf{x} + (1-\xi)\mathbf{y})(\mathbf{y} - \mathbf{x}). \tag{A.1.7}$$

We note that this mean-value theorem is simply the usual one for functions of a single variable as applied to the function

$$\hat{f}(t) = f(t\mathbf{x} + (1-t)\mathbf{y}).$$

If $f_1, \ldots, f_m$ are all functions of $n$ variables, then we denote the vector-valued function with components $f_1, \ldots, f_m$ by $\mathbf{F}$. For such vector-valued functions, there is a natural derivative defined by

$$\mathbf{F}'(\mathbf{x}) = \left(\frac{\partial f_i(\mathbf{x})}{\partial x_j}\right), \tag{A.1.8}$$

where the notation means that $\mathbf{F}'(\mathbf{x})$ is an $m \times n$ matrix, usually called the *Jacobian matrix*, whose $i$, $j$ element is the partial derivative of the $i$th component of $\mathbf{F}$ with respect to the $j$th variable. For example, if $m = n = 2$, then

$$\mathbf{F}'(\mathbf{x}) = \begin{bmatrix} \dfrac{\partial f_1(\mathbf{x})}{\partial x_1} & \dfrac{\partial f_1(\mathbf{x})}{\partial x_2} \\ \dfrac{\partial f_2(\mathbf{x})}{\partial x_1} & \dfrac{\partial f_2(\mathbf{x})}{\partial x_2} \end{bmatrix}.$$

Note that in the special case $m = 1$, $\mathbf{F}$ is simply the single function $f_1$, and the Jacobian matrix reduces to the row vector given by (A.1.6).

We next consider results for ordinary differential equations. If $y$ is a function of a single variable $t$, then an ordinary differential equation for $y$ is a relation of the form

$$F(t, y(t), y'(t), \ldots, y^{(n)}(t)) = 0 \tag{A.1.9}$$

for some given function $F$ of $n + 2$ variables, where the independent variable $t$ ranges over some finite or infinite interval. Equation (A.1.9) is the most general $n$th-order ordinary differential equation, where the *order* is determined by the highest-order derivative of the unknown function $y$ that appears in the equation. Usually the equation is assumed to be explicit in the highest derivative and is written as

$$y^{(n)}(t) = f(t, y, (t), y'(t), \ldots, y^{(n-1)}(t)). \tag{A.1.10}$$

If the function $f$ is linear in $y$ and its derivatives, then the equation is called linear and can be written in the form

$$y^{(n)}(t) = a_0(t) + a_1(t)y(t) + \cdots + a_n(t)y^{(n-1)}(t) \tag{A.1.11}$$

for given functions $a_0, \ldots, a_n$.

The equation (A.1.10) can also be considered for vector-valued functions $\mathbf{y}$ and $\mathbf{f}$, in which case we would have a system of $n$th-order equations. The simplest such possibility is a system of first-order equations

$$\mathbf{y}'(t) = \mathbf{f}(t, \mathbf{y}(t)), \tag{A.1.12}$$

where we assume that $\mathbf{y}$ and $\mathbf{f}$ are $n$ vectors with components $y_1, \ldots, y_n$ and $f_1, \ldots, f_n$.

In principle, a system of first-order equations is all that we need to consider, since a single $n$th-order equation can be reduced to a system of $n$ first-order equations (and, consequently, a system of $m$ $n$th-order equations to a system of $nm$ first-order equations). This reduction can be achieved, for example, as follows. Define new variables

$$y_i(t) \equiv y^{(i-1)}(t), \qquad i = 1, \ldots, n. \tag{A.1.13}$$

In terms of these variables, (A.1.10) becomes

$$y_n' = f(t, y_1, y_2, \ldots, y_{n-1}), \tag{A.1.14}$$

whereas from (A.1.13) we obtain

$$y_i' = y_{i+1}, \qquad i = 1, \ldots, n-1. \tag{A.1.15}$$

Equations (A.1.14), (A.1.15) give a first-order system of equations in the unknowns $y_1, \ldots, y_n$, where the component $y_1$ is the original unknown $y$ of equation (A.1.10).

A very important special case of (A.1.12) is when $\mathbf{f}$ is linear in $\mathbf{y}$, and the equation takes the form

$$\mathbf{y}'(t) = A(t)\mathbf{y}(t) + \mathbf{b}(t), \tag{A.1.16}$$

where $A$ is a given $n \times n$ matrix whose elements are functions of $t$, and $\mathbf{b}$ is a given vector function of $t$. An important special case of (A.1.16), in turn, is when $A$ is independent of $t$, and $\mathbf{b} = 0$, so that the equation is

$$\mathbf{y}' = A\mathbf{y}. \tag{A.1.17}$$

Such a *linear homogeneous* system with *constant coefficients* can, in principle, be solved explicitly by the series expansion

$$\mathbf{y}(t) = (I + At + \tfrac{1}{2}A^2t^2 + \cdots)\mathbf{c}, \tag{A.1.18}$$

where $\mathbf{c}$ is an arbitrary constant vector. The series expansion is simply that of the exponential of a matrix, and (A.1.18) can be written in the compact form

$$\mathbf{y}(t) = e^{At}\mathbf{c}. \tag{A.1.19}$$

Equation (A.1.19) shows that the general solution of (A.1.17) depends on $n$ arbitrary constants – the $n$ components of the vector $\mathbf{c}$. Thus, to obtain a unique solution of the system (A.1.17) $n$ additional conditions must be specified, and these are usually given in terms of *initial* or *boundary conditions*. For example, suppose that we desire a solution of (A.1.17) for $t \geq 0$ such that at $t = 0$ the solution takes on the initial condition $\mathbf{y}_0$. The solution is then given by (A.1.19) as $\mathbf{y}(t) = e^{At}\mathbf{y}_0$.

For more complicated equations the initial condition will not be represented in the solution in such a straightforward fashion. Indeed, it is not immediately obvious under what conditions the general *initial-value problem*

$$\mathbf{y}'(t) = \mathbf{f}(t, \mathbf{y}(t)), \qquad \mathbf{y}(0) = \mathbf{y}_0 \tag{A.1.20}$$

will even have a unique solution, but a number of basic theorems in this regard are known and may be found in any book on ordinary differential equations.

# Appendix 2

# Linear Algebra

The most important tool in many areas of scientific computing is linear algebra, and we review here some of the basic results that will be used.

If $A = (a_{ij})$ is a real $n \times n$ matrix, we denote the inverse of $A$ by $A^{-1}$ and the determinant by $\det A$. If the inverse of $A$ exists, then $A$ is *nonsingular*. The following basic result gives various other ways of stating this.

THEOREM A.2.1 *The following are equivalent:*

1. *$A$ is nonsingular.*
2. $\det A \neq 0$.
3. *The linear system $A\mathbf{x} = 0$ has only the solution $\mathbf{x} = 0$.*
4. *For any vector $\mathbf{b}$, the linear system $A\mathbf{x} = \mathbf{b}$ has a unique solution.*
5. *The columns (rows) of $A$ are linearly independent; that is, if $\mathbf{a}_1, \ldots, \mathbf{a}_n$ are the columns of $A$ and $\alpha_1\mathbf{a}_1 + \cdots + \alpha_n\mathbf{a}_n = 0$, then the scalars $\alpha_i$ are necessarily zero.*

The last condition may be rephrased to say that $A$ has rank $n$ where, in general, the *rank* is defined as the number of linearly independent columns (or rows) of the matrix.

The *transpose* of $A = (a_{ij})$ is $A^T = (a_{ji})$. A basic fact about determinants is that $\det A^T = \det A$. Thus, by **2.** of Theorem A.2.1, $A^T$ is nonsingular if and only if $A$ is nonsingular. A particularly important type of matrix satisfies $A^T = A$ and is called *symmetric*. If, in addition, $\mathbf{x}^T A\mathbf{x} > 0$ for $\mathbf{x} \neq 0$, then $A$ is *positive definite*. By **3.** of Theorem A.2.1, a positive definite matrix is nonsingular.

A *submatrix* of $A$ is obtained by deleting rows and columns of $A$. A *principle* submatrix results from deleting corresponding rows and columns; in particular, a *leading* principle submatrix of size $k$ is obtained by deleting rows and columns $k+1, k+2, \ldots$. An important fact is that any principle submatrix of a symmetric positive definite matrix is also symmetric positive definite.

Section 7.1 is devoted to a review of eigenvalues and we give in this appendix only the basic facts. A (real or complex) scalar $\lambda$ and a vector $\mathbf{x} \neq 0$ are an *eigenvalue* and *eigenvector*, respectively, of the matrix $A$ if

$$A\mathbf{x} = \lambda\mathbf{x}. \tag{A.2.1}$$

By Theorem A.2.1, it follows that $\lambda$ is an eigenvalue if and only if

$$\det(A - \lambda I) = 0. \tag{A.2.2}$$

This is the *characteristic equation* of $A$ and is a polynomial of degree $n$ in $\lambda$. (Here, as always, $I$ is the identity matrix.) Consequently, $A$ has precisely $n$ (not necessarily distinct) eigenvalues – the $n$ roots of (A.2.2). The collection of these $n$ eigenvalues $\lambda_1, \cdots, \lambda_n$ is called the *spectrum* of $A$, and

$$\rho(A) = \max_{1 \leq i \leq n} |\lambda_i| \tag{A.2.3}$$

is the *spectral radius* of $A$. Even if the matrix $A$ is real, the eigenvalues of $A$ may be complex. If $A$ is symmetric, however, then its eigenvalues are necessarily real. Moreover, if $A$ is also positive-definite, then its eigenvalues are also positive. The converse also holds; that is, if all the eigenvalues of a symmetric matrix are positive, then the matrix is positive-definite.

Eigenvalues are generally difficult to compute, but there is an important class of matrices in which they are available by inspection. These are upper- or lower- *triangular matrices*

$$A = \begin{bmatrix} a_{11} & \cdots & a_{1n} \\ & \ddots & \vdots \\ & & a_{nn} \end{bmatrix}, \qquad A = \begin{bmatrix} a_{11} & & \\ \vdots & \ddots & \\ a_{n1} & \cdots & a_{nn} \end{bmatrix},$$

for which the eigenvalues are simply the main diagonal elements. An important special case of triangular matrices are *diagonal matrices*

$$D = \begin{bmatrix} d_1 & & \\ & \ddots & \\ & & d_n \end{bmatrix},$$

which we will usually denote by $D = \text{diag}(d_1, \ldots, d_n)$.

The Euclidean length of a vector $\mathbf{x}$ is defined by

$$||\mathbf{x}||_2 = \left( \sum_{i=1}^{n} x_i^2 \right)^{1/2}. \tag{A.2.4}$$

This is a special case of a *vector norm*, which is a real-valued function that satisfies the following distance-like properties:

1. $||\mathbf{x}|| \geq 0$ for any vector $\mathbf{x}$ and $||\mathbf{x}|| = 0$ only if $\mathbf{x} = 0$.
2. $||\alpha\mathbf{x}|| = |\alpha| \, ||\mathbf{x}||$ for any scalar $\alpha$. (A.2.5)
3. $||\mathbf{x} + \mathbf{y}|| \leq ||\mathbf{x}|| + ||\mathbf{y}||$ for all vectors $\mathbf{x}$ and $\mathbf{y}$.

Property 3 is known as the *triangle inequality.*

The Euclidean length (A.2.4) satisfies these properties and is usually called the Euclidean norm, or $l_2$ norm. Other commonly used norms are defined by

$$||\mathbf{x}||_1 = \sum_{i=1}^{n} |x_i|, \qquad ||\mathbf{x}||_\infty = \max_{1 \leq i \leq n} |x_i|, \tag{A.2.6}$$

which are known as the $l_1$ norm, and the $l_\infty$ or max norm, respectively. The three norms (A.2.4) and (A.2.6) are special cases of the general class of $l_p$ norms

$$||\mathbf{x}||_p = \left( \sum_{i=1}^{n} |x_i^p| \right)^{1/p}, \tag{A.2.7}$$

defined for any real number $p \in [1, \infty)$. The $l_\infty$ norm is the limiting case of (A.2.7) as $p \to \infty$. Another important class of norms consists of the *elliptic norms* defined by

$$||\mathbf{x}|| = (\mathbf{x}^T B \mathbf{x})^{1/2}$$

for some given symmetric positive-definite matrix $B$; the Euclidean norm is the special case $B = I$.

These various norms can be visualized geometrically in terms of the set of vectors $\{\mathbf{x} : ||\mathbf{x}|| = 1\}$, which is known as the *unit sphere.* These are shown in Figure A.2.1 for vectors in the plane. Note that only for the Euclidean norm are the unit vectors on the circle of radius 1.

The elliptic norms play a particularly central role in matrix theory because they arise in terms of an *inner product*, which in turn defines orthogonality of vectors. An inner product is a real-valued function of two vector variables that satisfies the following conditions (stated only for real vectors):

1. $(\mathbf{x}, \mathbf{x}) \geq 0$ for all vectors $x$; $(\mathbf{x}, \mathbf{x}) = 0$ only if $\mathbf{x} = 0$.
2. $(\alpha\mathbf{x}, \mathbf{y}) = \alpha(\mathbf{x}, \mathbf{y})$ for all vectors $\mathbf{x}$ and $\mathbf{y}$ and scalars $\alpha$.
3. $(\mathbf{x}, \mathbf{y}) = (\mathbf{y}, \mathbf{x})$ for all vectors $\mathbf{x}$ and $\mathbf{y}$. (A.2.8)
4. $(\mathbf{x} + \mathbf{z}, \mathbf{y}) = (\mathbf{x}, \mathbf{y}) + (\mathbf{z}, \mathbf{y})$ for all vectors $\mathbf{x}$, $\mathbf{y}$, and $\mathbf{z}$.

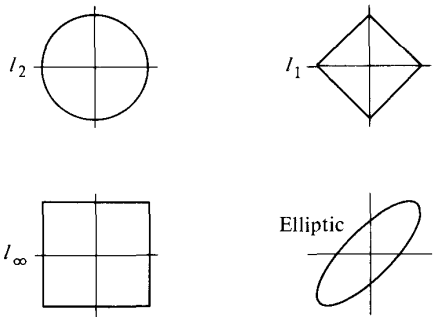


Figure A.2.1: *Unit Spheres of Several Norms*

For any inner product a norm may be defined by

$$||\mathbf{x}|| = (\mathbf{x}, \mathbf{x})^{1/2},$$

and the elliptic norms then derive from the inner product

$$(\mathbf{x}, \mathbf{y}) \equiv \mathbf{x}^T B \mathbf{y}. \tag{A.2.9}$$

Two nonzero vectors $\mathbf{x}$ and $\mathbf{y}$ are *orthogonal* with respect to some inner product if

$$(\mathbf{x}, \mathbf{y}) = 0.$$

If the inner product is the Euclidean one defined by (A.2.9) with $B = I$, then this gives the usual and intuitive concept of orthogonality. A set of nonzero vectors $\mathbf{x}_1, \ldots, \mathbf{x}_m$ is *orthogonal* if

$$(\mathbf{x}_i, \mathbf{x}_j) = 0, \qquad i \neq j.$$

A set of orthogonal vectors is necessarily linearly independent, and a set of $n$ such vectors is said to be an *orthogonal basis.* If, in addition, $||\mathbf{x}_i||_2 = 1, \quad i = 1, \cdots, n$, the vectors are *orthonormal.*

If the columns of a matrix $A$ are orthonormal in the inner product $\mathbf{x}^T\mathbf{y}$,then $A^T A = I$ and the matrix is *orthogonal.* Orthogonal matrices have the important property that they preserve the length of a vector; that is, $||A\mathbf{x}||_2 = ||\mathbf{x}||_2$.

Convergence of a sequence of vectors $\{\mathbf{x}^k\}$ to a limit vector $\mathbf{x}$ is defined in terms of a norm by

$$||\mathbf{x}^k - \mathbf{x}|| \to 0 \qquad \text{as} \qquad k \to \infty.$$

It is natural to suppose that a sequence might converge in one norm but not in another. Surprisingly, this cannot happen.

THEOREM A.2.2: *The following are equivalent:*

1. *The sequence* $\{\mathbf{x}^k\}$ *converges to* $\mathbf{x}$ *in some norm.*
2. *The sequence* $\{\mathbf{x}^k\}$ *converges to* $\mathbf{x}$ *in every norm.*
3. *The components of the sequence* $\{\mathbf{x}^k\}$ *all converge to the corresponding components of* $\mathbf{x}$*; that is,* $x_i^k \to x_i$ *as* $k \to \infty$ *for* $i = 1, \ldots, n$.

As a consequence of this result – sometimes known as the *norm equivalence theorem* – when we speak of the convergence of a sequence of vectors, it is immaterial whether or not we specify the norm.

Any vector norm gives rise to a corresponding matrix norm by means of the definition

$$||A|| = \max_{\mathbf{x} \neq 0} \frac{||A\mathbf{x}||}{||\mathbf{x}||} = \max_{||\mathbf{x}||=1} ||A\mathbf{x}||. \tag{A.2.10}$$

The properties (A.2.5) also hold for a matrix norm; in addition, there is the multiplicative property $||AB|| \leq ||A||\ ||B||$. The geometric interpretation of a matrix norm is that $||A||$ is the maximum length of a unit vector after transformation by $A$; this is depicted in Figure A.2.2 for the $l_2$ norm.

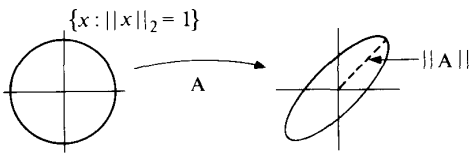


Figure A.2.2: *The* $l_2$ *Norm*

As with vectors, the convergence of a sequence of matrices may be defined component-wise or, equivalently, in terms of any matrix norm. That is, we write $A_k \to A$ as $k \to \infty$ if in some norm $||A_k - A|| \to 0$ as $k \to \infty$. Again, convergence in some norm implies convergence in any norm.

The matrix norms corresponding to the $l_1$ and $l_\infty$ vector norms are easily computed by

$$||A||_1 = \max_{1 \leq j \leq n} \sum_{i=1}^{n} |a_{ij}|, \qquad ||A||_\infty = \max_{1 \leq i \leq n} \sum_{j=1}^{n} |a_{ij}|. \tag{A.2.11}$$

That is, $||A||_1$ is the maximum absolute value column sum of the elements of $A$, and $||A||_\infty$ is the maximum row sum. The Euclidean matrix norm is given in terms of the spectral radius of $A^TA$ by

$$||A||_2 = [\rho(A^TA)]^{1/2} \tag{A.2.12}$$

and is much more difficult to compute. If $A$ is symmetric, (A.2.12) reduces to

$$||A||_2 = \rho(A), \tag{A.2.13}$$

which is still difficult to compute but is more directly related to the matrix $A$.

We note that it follows immediately from (A.2.10) that if $\lambda$ is any eigenvalue of $A$ and $\mathbf{x}$ a corresponding eigenvector, then

$$|\lambda| \, ||\mathbf{x}|| = ||\lambda\mathbf{x}|| = ||A\mathbf{x}|| \leq ||A|| \, ||\mathbf{x}||,$$

so that $|\lambda| \leq ||A||$; thus, any norm of the matrix $A$ gives a bound on all eigenvalues of $A$. In general, however, the property (A.2.13) of the $l_2$ norm will not hold.