Appendix: Useful Mathematical Techniques

This appendix contains concise reviews of various mathematical techniques used in this book. We start with formulae useful for solving triangles, both planar and spherical. Next, some aspects of the manipulation of vectors are summarized. These include solution methods for vector equations and conventions for differentiation with respect to a vector and a matrix. Least-squares methods for linear systems come next. These are followed by a review of optimization methods, both unconstrained and constrained. The appendix ends with a look at the calculus of variations.

A.1 Solving Triangles

Suppose a planar triangle has sides a, b, and c with opposite angles A, B, and C (figure A-1a). The diameter of the circumscribed circle equals the length of one side divided by the sine of the opposite angle. Since this is true for all three choices of sides, we have

$$\frac{a}{\sin A} = \frac{b}{\sin B} = \frac{c}{\sin C}.$$

This is the well-known *law of sines*. The *law of cosines* is given by

$$a^2 = b^2 + c^2 - 2bc \cos A.$$

Two similar formulae can be obtained by simultaneous cyclical permutation of a, b, c and A, B, C. The *projection theorem* states that

$$c = a \cos B + b \cos A.$$

(There are many other useful relationships, but we can usually manage with just these three; others can be derived from them if necessary.) The area of the triangle can be written

$$S = \frac{1}{2} ab \sin C.$$

A *spherical triangle* is a figure on the sphere whose three sides are segments of great circles (figure A-1b). Suppose that the angles of intersection at the three corners are A, B, and C. On the unit sphere, the length of a side is equal to the angle it subtends at the center of the sphere. Let the lengths of the three sides be a, b, and c. In the case of a spherical triangle, the law of sines is

$$\frac{\sin a}{\sin A} = \frac{\sin b}{\sin B} = \frac{\sin c}{\sin C}.$$

The law of cosines for the sides is

$$\cos a = \cos b \cos c + \sin b \sin c \cos A,$$

while the law of cosines for the angles is

$$\cos A = -\cos B \cos C + \sin B \sin C \cos a.$$

There are two more formulae in each case obtained by simultaneous cyclical permutation of a, b, c and A, B, C. (Other relations can be derived from these if necessary.)

Sometimes it is difficult to determine which quadrant an angle lies in. In this case, the *rule of quadrants* comes to the rescue: $\frac{1}{2}(A + B)$ is in the same quadrant as $\frac{1}{2}(a + b)$. Finally, we note that the area of a spherical triangle is

$$S_R = R^2 \epsilon.$$

Here R is the radius of the sphere, while $\epsilon = A + B + C - \pi$ is called the *spherical excess* (measured in radians).

A.2 Manipulation of Vectors

We shall assume that the reader is familiar with the properties of vector addition, scalar multiplication, and dot- and cross-products. Vectors will be denoted by boldface letters. We commonly deal with column vectors and therefore have to take the transpose, indicated by the superscript ^{T}, when we want to write them in terms of the equivalent row vectors.

A.2.1 More Complex Products of Vectors

The vector *triple product* is defined as follows:

$$[\mathbf{a}\,\mathbf{b}\,\mathbf{c}] = \mathbf{a}\cdot(\mathbf{b}\times\mathbf{c}) = (\mathbf{a}\times\mathbf{b})\cdot\mathbf{c}.$$

The magnitude of the result is independent of the order of the vectors, since it is the volume of the parallelepiped defined by the three vectors. The sign of the result is the same for all triple products with the same cyclical order. If the three vectors lie in a plane, they are linearly dependent, and in this case the triple product is zero.

The following identities apply to other complicated products of vectors:

$$\mathbf{a}\times(\mathbf{b}\times\mathbf{c}) = (\mathbf{c}\cdot\mathbf{a})\mathbf{b} - (\mathbf{a}\cdot\mathbf{b})\mathbf{c},$$
$$(\mathbf{a}\times\mathbf{b})\times\mathbf{c} = (\mathbf{c}\cdot\mathbf{a})\mathbf{b} - (\mathbf{b}\cdot\mathbf{c})\mathbf{a}.$$

Thus we have

$$\big((\mathbf{a}\times\mathbf{b})\times\mathbf{c}\big)\cdot\mathbf{d} + \big((\mathbf{b}\times\mathbf{c})\times\mathbf{a}\big)\cdot\mathbf{d} + \big((\mathbf{c}\times\mathbf{a})\times\mathbf{b}\big)\cdot\mathbf{d} = 0,$$

$$\mathbf{a}\times\big(\mathbf{b}\times(\mathbf{c}\times\mathbf{d})\big) = (\mathbf{b}\cdot\mathbf{d})(\mathbf{c}\times\mathbf{a}) - (\mathbf{b}\cdot\mathbf{c})(\mathbf{d}\times\mathbf{a}),$$

$$(\mathbf{a}\times\mathbf{b})\cdot(\mathbf{c}\times\mathbf{d}) = (\mathbf{c}\cdot\mathbf{a})(\mathbf{b}\cdot\mathbf{d}) - (\mathbf{d}\cdot\mathbf{a})(\mathbf{b}\cdot\mathbf{c}),$$

and from these we can derive

$$(\mathbf{a}\times\mathbf{b})\cdot(\mathbf{c}\times\mathbf{d})+(\mathbf{b}\times\mathbf{c})\cdot(\mathbf{a}\times\mathbf{d})+(\mathbf{c}\times\mathbf{a})\cdot(\mathbf{b}\times\mathbf{d})=0,$$

$$|\mathbf{a}\times\mathbf{b}|^2=|\mathbf{a}|^2\,|\mathbf{b}|^2-(\mathbf{a}\cdot\mathbf{b})^2.$$

Note that this last quantity cannot be negative. Also,

$$(\mathbf{a}\times\mathbf{b})\times(\mathbf{c}\times\mathbf{d})=[\mathbf{d}\,\mathbf{a}\,\mathbf{b}]\mathbf{c}-[\mathbf{a}\,\mathbf{b}\,\mathbf{c}]\mathbf{d},$$

$$(\mathbf{a}\times\mathbf{b})\times(\mathbf{c}\times\mathbf{d})=[\mathbf{c}\,\mathbf{d}\,\mathbf{a}]\mathbf{b}-[\mathbf{b}\,\mathbf{c}\,\mathbf{d}]\mathbf{a}.$$

From this it follows that

$$\big[(\mathbf{a}\times\mathbf{b})\ (\mathbf{c}\times\mathbf{d})\ (\mathbf{e}\times\mathbf{f})\big]=[\mathbf{d}\,\mathbf{a}\,\mathbf{b}]\,[\mathbf{c}\,\mathbf{e}\,\mathbf{f}]-[\mathbf{a}\,\mathbf{b}\,\mathbf{c}]\,[\mathbf{d}\,\mathbf{e}\,\mathbf{f}],$$

and so

$$\big[(\mathbf{a}\times\mathbf{b})\ (\mathbf{b}\times\mathbf{c})\ (\mathbf{c}\times\mathbf{a})\big]=[\mathbf{a}\,\mathbf{b}\,\mathbf{c}]^2.$$

We can express any given vector $\mathbf{d}$ in terms of any three independent vectors $\mathbf{a}$, $\mathbf{b}$, and $\mathbf{c}$:

$$[\mathbf{a}\,\mathbf{b}\,\mathbf{c}]\mathbf{d}=[\mathbf{b}\,\mathbf{c}\,\mathbf{d}]\mathbf{a}+[\mathbf{d}\,\mathbf{c}\,\mathbf{a}]\mathbf{b}+[\mathbf{d}\,\mathbf{a}\,\mathbf{b}]\mathbf{c}.$$

This identity can be used to solve linear vector equations.

A.2.2 Solving Vector Equations

Suppose we are to find a vector $\mathbf{x}$ given its dot-products with three known linearly independent vectors, $\mathbf{a}$, $\mathbf{b}$, and $\mathbf{c}$. We have

$$\mathbf{x}\cdot\mathbf{a}=\alpha,\qquad \mathbf{x}\cdot\mathbf{b}=\beta,\qquad \text{and}\qquad \mathbf{x}\cdot\mathbf{c}=\gamma.$$

The unknown $\mathbf{x}$ can be expressed in terms of any three independent vectors. Rather than use $\mathbf{a}$, $\mathbf{b}$, and $\mathbf{c}$ for this purpose, consider a linear combination of their pairwise cross-products:

$$\mathbf{x}=u(\mathbf{b}\times\mathbf{c})+v(\mathbf{c}\times\mathbf{a})+w(\mathbf{a}\times\mathbf{b}).$$

It remains for us to determine the three scalars u, v, and w. Taking the dot-product of the above expression with the three vectors $\mathbf{a}$, $\mathbf{b}$, and $\mathbf{c}$, we obtain

$$u[\mathbf{a}\,\mathbf{b}\,\mathbf{c}]=\alpha,\qquad v[\mathbf{a}\,\mathbf{b}\,\mathbf{c}]=\beta,\quad \text{and}\quad w[\mathbf{a}\,\mathbf{b}\,\mathbf{c}]=\gamma.$$

Thus we have

$$\mathbf{x}=\frac{1}{[\mathbf{a}\,\mathbf{b}\,\mathbf{c}]}\big(\alpha(\mathbf{b}\times\mathbf{c})+\beta(\mathbf{c}\times\mathbf{a})+\gamma(\mathbf{a}\times\mathbf{b})\big).$$

The same result could have been obtained by noting that

$$[\mathbf{a}\,\mathbf{b}\,\mathbf{c}]\mathbf{x} = (\mathbf{b}\times\mathbf{c})(\mathbf{a}\cdot\mathbf{x}) + (\mathbf{c}\times\mathbf{a})(\mathbf{b}\cdot\mathbf{x}) + (\mathbf{a}\times\mathbf{b})(\mathbf{c}\cdot\mathbf{x}).$$

The above method amounts to solving three equations in three unknowns. The result can therefore be used in inverting a 3×3 matrix $\mathbf{M}$ that has the vectors $\mathbf{a}^T$, $\mathbf{b}^T$, and $\mathbf{c}^T$ as rows:

$$\mathbf{M} = \begin{pmatrix} \mathbf{a}^T \\ \mathbf{b}^T \\ \mathbf{c}^T \end{pmatrix}.$$

The determinant of this matrix is just $[\mathbf{a}\,\mathbf{b}\,\mathbf{c}]$. According to the previous result, the inverse of this matrix is just the matrix of column vectors obtained by taking the pairwise cross-products, divided by the value of the determinant:

$$\mathbf{M}^{-1} = \frac{1}{[\mathbf{a}\,\mathbf{b}\,\mathbf{c}]}\big((\mathbf{b}\times\mathbf{c})\ (\mathbf{c}\times\mathbf{a})\ (\mathbf{a}\times\mathbf{b})\big).$$

The result is easily checked by matrix multiplication. There is a symmetric form of this result in which the columns rather than the rows of the original matrix are considered as vectors.

We turn now to other vector equations. Given an equation

$$\lambda\mathbf{x} + \mathbf{x}\times\mathbf{a} = \mathbf{b},$$

we want to find the unknown $\mathbf{x}$. It can be shown that

$$\lambda(\mathbf{b}-\lambda\mathbf{x}) + \lambda^{-1}(\mathbf{b}\cdot\mathbf{a})\mathbf{a} - a^2\mathbf{x} = \mathbf{b}\times\mathbf{a},$$

so that

$$\mathbf{x} = \frac{\lambda\mathbf{b} + \lambda^{-1}(\mathbf{b}\cdot\mathbf{a})\mathbf{a} - \mathbf{b}\times\mathbf{a}}{\lambda^2 + a^2},$$

provided $\lambda \neq 0$.

Given another vector equation,

$$\lambda\mathbf{x} + (\mathbf{x}\cdot\mathbf{b})\mathbf{a} = \mathbf{c},$$

we again want to find $\mathbf{x}$. Taking the dot-product with $\mathbf{b}$, we get

$$(\mathbf{x}\cdot\mathbf{b})\big(\lambda + \mathbf{a}\cdot\mathbf{b}\big) = \mathbf{b}\cdot\mathbf{c},$$

so that

$$\mathbf{x} = \frac{1}{\lambda}\left(\mathbf{c} - \mathbf{a}\frac{\mathbf{b}\cdot\mathbf{c}}{\lambda + \mathbf{a}\cdot\mathbf{b}}\right),$$

provided $\lambda + \mathbf{a} \cdot \mathbf{b} \neq 0$.

Next, consider finding a vector $\mathbf{x}$, given its size and its dot-products with two test vectors $\mathbf{a}$ and $\mathbf{b}$. Thus

$$\mathbf{a} \cdot \mathbf{x} = \alpha, \qquad \mathbf{b} \cdot \mathbf{x} = \beta, \qquad \text{and} \qquad \mathbf{x} \cdot \mathbf{x} = \gamma.$$

Unless $\mathbf{a}$ and $\mathbf{b}$ are parallel, we know that $\mathbf{a}$, $\mathbf{b}$, and $\mathbf{a} \times \mathbf{b}$ are linearly independent. Thus the unknown vector can be expressed as

$$\mathbf{x} = u\mathbf{a} + v\mathbf{b} + w(\mathbf{a} \times \mathbf{b}).$$

We can find u and v from

$$|\mathbf{a} \times \mathbf{b}|^2 \, u = +\alpha(\mathbf{b} \cdot \mathbf{b}) - \beta(\mathbf{a} \cdot \mathbf{b}),$$

$$|\mathbf{a} \times \mathbf{b}|^2 \, v = -\alpha(\mathbf{a} \cdot \mathbf{b}) + \beta(\mathbf{a} \cdot \mathbf{a}).$$

Moreover,

$$|\mathbf{a} \times \mathbf{b}|^2 \,(u\mathbf{a} + v\mathbf{b}) = \big[(\mathbf{b} \cdot \mathbf{b})\mathbf{a} - (\mathbf{a} \cdot \mathbf{b})\mathbf{b}\big]\alpha - \big[(\mathbf{a} \cdot \mathbf{b})\mathbf{a} - (\mathbf{a} \cdot \mathbf{a})\mathbf{b}\big]\beta,$$

and so

$$|\mathbf{a} \times \mathbf{b}|^2 \,|u\mathbf{a} + v\mathbf{b}|^2 = |\mathbf{a} \times \mathbf{b}|^2 \,(u\mathbf{a} + v\mathbf{b}) \cdot \mathbf{c} = |\beta\mathbf{a} - \alpha\mathbf{b}|^2 .$$

Now

$$\mathbf{x} \cdot \mathbf{x} = |u\mathbf{a} + v\mathbf{b}|^2 + w^2 \,|\mathbf{a} \times \mathbf{b}|^2 ,$$

or

$$|\mathbf{a} \times \mathbf{b}|^4 \, w^2 = |\mathbf{a} \times \mathbf{b}|^2 \,\gamma - |\beta\mathbf{a} - \alpha\mathbf{b}|^2 .$$

We thus obtain the two solutions

$$w = \pm \frac{\sqrt{|\mathbf{a} \times \mathbf{b}|^2 \,\gamma - |\beta\mathbf{a} - \alpha\mathbf{b}|^2}}{|\mathbf{a} \times \mathbf{b}|^2}.$$

A.3 Vector and Matrix Differentiation

Often a set of equations can be written more compactly in vector notation. The advantage of this may evaporate when it becomes necessary to look at the derivatives of a scalar or vector with respect to the components of a vector. It is, however, possible to use a consistent, compact notation in this case also.

A.3.1 Differentiation of a Scalar with Respect to a Vector

The derivative of a scalar with respect to a vector is the vector whose components are the derivatives of the scalar with respect to each of the components of the vector. If $\mathbf{r} = (x, y, z)^T$, then

$$\frac{df}{d\mathbf{r}} = (f_x, f_y, f_z)^T .$$

Consequently,

$$\frac{d}{d\mathbf{a}}(\mathbf{a} \cdot \mathbf{b}) = \mathbf{b} \quad \text{and} \quad \frac{d}{d\mathbf{b}}(\mathbf{a} \cdot \mathbf{b}) = \mathbf{a}.$$

The length of a vector is the square root of the sum of the squares of its elements,

$$|\mathbf{a}| = \sqrt{\mathbf{a} \cdot \mathbf{a}}.$$

We see that

$$\frac{d}{d\mathbf{a}} |\mathbf{a}|^2 = 2\mathbf{a},$$

so that

$$\frac{d}{d\mathbf{a}} |\mathbf{a}| = \hat{\mathbf{a}},$$

where $\hat{\mathbf{a}} = \mathbf{a}/ |\mathbf{a}|$; also,

$$\frac{d}{d\mathbf{a}}[\mathbf{a}\,\mathbf{b}\,\mathbf{c}] = \mathbf{b} \times \mathbf{c},$$

where $[\mathbf{a}\,\mathbf{b}\,\mathbf{c}] = \mathbf{a} \cdot (\mathbf{b} \times \mathbf{c})$ as before. Furthermore,

$$\frac{d}{d\mathbf{a}}\mathbf{a}^T\mathbf{M}\mathbf{b} = \mathbf{M}\mathbf{b} \qquad \text{and} \qquad \frac{d}{d\mathbf{b}}\mathbf{a}^T\mathbf{M}\mathbf{b} = \mathbf{M}^T\mathbf{a}.$$

In particular,

$$\frac{d}{d\mathbf{x}}\mathbf{x}^T\mathbf{M}\mathbf{x} = (\mathbf{M} + \mathbf{M}^T)\mathbf{x}.$$

The derivative of a scalar with respect to a matrix is the matrix whose components are the derivatives of the scalar with respect to the elements of the matrix. Thus if

$$\mathbf{M} = \begin{pmatrix} a & b \\ c & d \end{pmatrix},$$

then

$$\frac{df}{d\mathbf{M}} = \begin{pmatrix} \frac{df}{da} & \frac{df}{db} \\ \frac{df}{dc} & \frac{df}{dd} \end{pmatrix}.$$

Consequently,

$$\frac{d}{d\mathbf{M}}\text{Trace}(\mathbf{M}) = I,$$

where the trace of a matrix is the sum of its diagonal elements and I is the identity matrix. Also,

$$\frac{d}{d\mathbf{M}}\mathbf{a}^T\mathbf{M}\mathbf{b} = \mathbf{a}\,\mathbf{b}^T.$$

In particular,

$$\frac{d}{d\mathbf{M}}\mathbf{x}^T\mathbf{M}\mathbf{x} = \mathbf{x}\,\mathbf{x}^T.$$

Note that $\mathbf{a}\,\mathbf{b}^T$ is not the scalar $\mathbf{a}\cdot\mathbf{b}$. The latter equals $\mathbf{a}^T\mathbf{b}$. If $\mathbf{a} = (a_x, a_y, a_z)^T$ and $\mathbf{b} = (b_x, b_y, b_z)^T$, the *dyadic product* is

$$\mathbf{a}\,\mathbf{b}^T = \begin{pmatrix} a_x b_x & a_x b_y & a_x b_z \\ a_y b_x & a_y b_y & a_y b_z \\ a_z b_x & a_z b_y & a_z b_z \end{pmatrix}.$$

Another interesting matrix derivative is

$$\frac{d}{d\mathbf{M}}\text{Det}(\mathbf{M}) = \text{Det}(\mathbf{M})\,(\mathbf{M}^{-1})^T.$$

That this is the matrix of cofactors can be shown as follows. Consider a particular element m_{ij} of the matrix $\mathbf{M}$. We can express the determinant as the sum

$$\text{Det}(\mathbf{M}) = \sum_{k=1}^{n} m_{ik}c_{ik}$$

by expanding along the row containing this element, where c_{ij} is the cofactor of m_{ij}. Thus the derivative of the determinant with respect to m_{ij} is just c_{ij}. (The cofactor c_{ij} is $(-1)^{i+j}$ times the determinant of the matrix obtained by deleting the i^{th} row and the j^{th} column.) The result follows from the fact that the inverse of a matrix equals the transpose of the matrix of cofactors divided by the value of the determinant.

Next, if $\mathbf{A}$ and $\mathbf{B}$ are compatible matrices (that is, if $\mathbf{A}$ has as many columns as $\mathbf{B}$ has rows), then

$$\frac{d}{d\mathbf{A}}\text{Trace}(\mathbf{A}\,\mathbf{B}) = \mathbf{B}^T \quad \text{and} \quad \frac{d}{d\mathbf{B}}\text{Trace}(\mathbf{A}\,\mathbf{B}) = \mathbf{A}^T.$$

Also, in general,

$$\frac{d}{d\mathbf{M}}\text{Trace}(\mathbf{A}\,\mathbf{M}\,\mathbf{B}) = \mathbf{A}^T\mathbf{B}^T.$$

One norm of a matrix is the square root of the sum of squares of its elements:

$$\|\mathbf{M}\|^2 = \text{Trace}(\mathbf{M}^T\mathbf{M}).$$

We see that

$$\frac{d}{d\mathbf{M}}\|\mathbf{M}\|^2 = 2\,\mathbf{M},$$

and it follows from

$$\|\mathbf{A}-\mathbf{B}\|^2 = \text{Trace}(\mathbf{A}^T\mathbf{A} - \mathbf{B}^T\mathbf{A} - \mathbf{A}^T\mathbf{B} + \mathbf{B}^T\mathbf{B})$$

or

$$\|\mathbf{A}-\mathbf{B}\|^2 = \|\mathbf{A}\|^2 - 2\,\text{Trace}(\mathbf{A}^T\mathbf{B}) + \|\mathbf{B}\|^2$$

that

$$\frac{d}{d\mathbf{A}}\|\mathbf{A}-\mathbf{B}\|^2 = 2(\mathbf{A}-\mathbf{B}) \quad \text{and} \quad \frac{d}{d\mathbf{B}}\|\mathbf{A}-\mathbf{B}\|^2 = 2(\mathbf{B}-\mathbf{A}).$$

A.3.2 Differentiation of a Vector with Respect to a Vector

Occasionally it is also useful to define a matrix that contains as elements the derivatives of the components of one vector with respect to the components of another:

$$\frac{d\mathbf{b}}{d\mathbf{a}} = \begin{pmatrix} \frac{db_x}{da_x} & \frac{db_x}{da_y} & \frac{db_x}{da_z} \\ \frac{db_y}{da_x} & \frac{db_y}{da_y} & \frac{db_y}{da_z} \\ \frac{db_z}{da_x} & \frac{db_z}{da_y} & \frac{db_z}{da_z} \end{pmatrix}.$$

This matrix is just the Jacobian $\mathbf{J}$ of the coordinate transformation from $\mathbf{a}$ to $\mathbf{b}$. Clearly,

$$\frac{d}{d\mathbf{a}}\mathbf{M}\mathbf{a} = \mathbf{M}$$

for any matrix $\mathbf{M}$. We also see that

$$\frac{d}{d\mathbf{b}}(\mathbf{a}\times\mathbf{b}) = \begin{pmatrix} 0 & -a_z & +a_y \\ +a_z & 0 & -a_x \\ -a_y & +a_x & 0 \end{pmatrix},$$

and so conclude that

$$\mathbf{a}\times\mathbf{b} = \begin{pmatrix} 0 & -a_z & +a_y \\ +a_z & 0 & -a_x \\ -a_y & +a_x & 0 \end{pmatrix}\mathbf{b}.$$

This defines an isomorphism between vectors and antisymmetric matrices that can be useful when we are dealing with cross-products.

A.4 Least-Squares Solutions of Linear Equations

Let $\mathbf{a} = \mathbf{M}\mathbf{b}$, where $\mathbf{M}$ is an $m \times n$ matrix, $\mathbf{a}$ is a vector with m components, and $\mathbf{b}$ is a vector with n components. Suppose that we have n measurements $\{\mathbf{a}_i\}$ and $\{\mathbf{b}_i\}$ and wish to calculate the matrix $\mathbf{M}$. We can form the matrices $\mathbf{A}$ and $\mathbf{B}$ by adjoining the vectors $\{\mathbf{a}_i\}$ and $\{\mathbf{b}_i\}$, respectively. (That is, the i^{th} column of the matrix $\mathbf{A}$ is $\mathbf{a}_i$.) Then

$$\mathbf{A} = \mathbf{M}\,\mathbf{B}.$$

Now $\mathbf{B}$ is a square matrix. If it has an inverse, then

$$\mathbf{M} = \mathbf{A}\,\mathbf{B}^{-1}.$$

Suppose that we have more measurements. The problem is then overdetermined, with more equations than unknowns. We can define an error vector $\mathbf{e}$ with m components

$$\mathbf{e}_i = \mathbf{a}_i - \mathbf{M}\mathbf{b}_i.$$

Adjoining these k vectors, we obtain

$$\mathbf{E} = \mathbf{A} - \mathbf{M}\,\mathbf{B}.$$

The sum of the squares of the errors is

$$\sum |\mathbf{e}_i|^2 = \sum \mathbf{e}_i \cdot \mathbf{e}_i = \sum \mathbf{e}_i^T \mathbf{e}_i,$$

or

$$\text{Trace}(\mathbf{E}^T\mathbf{E}) = \text{Trace}\big((\mathbf{A} - \mathbf{M}\,\mathbf{B})^T(\mathbf{A} - \mathbf{M}\,\mathbf{B})\big),$$

or

$$\text{Trace}(\mathbf{E}^T\mathbf{E}) = \text{Trace}(\mathbf{A}^T\mathbf{A} - \mathbf{B}^T\mathbf{M}^T\mathbf{A} - \mathbf{A}^T\mathbf{M}\,\mathbf{B} + \mathbf{B}^T\mathbf{M}^T\mathbf{M}\,\mathbf{B}).$$

Thus

$$\frac{d}{d\mathbf{M}}\text{Trace}(\mathbf{E}^T\mathbf{E}) = -\mathbf{A}\,\mathbf{B}^T - \mathbf{A}\,\mathbf{B}^T + (\mathbf{B}^T\mathbf{M}^T)^T\mathbf{B}^T + (\mathbf{B}^T\mathbf{M}^T)^T\mathbf{B}^T.$$

If this is to equal zero, then $\mathbf{A}\,\mathbf{B}^T = \mathbf{M}\,\mathbf{B}\,\mathbf{B}^T$, that is,

$$\mathbf{M} = \mathbf{A}\,\mathbf{B}^T(\mathbf{B}\,\mathbf{B}^T)^{-1}.$$

The term $\mathbf{B}^T(\mathbf{B}\,\mathbf{B}^T)^{-1}$ is called the *pseudoinverse* of the nonsquare matrix $\mathbf{B}$.

The problem is underdetermined, on the other hand, if there are fewer equations than unknowns. There are then infinitely many solutions. In this case the pseudoinverse provides the solution with least norm, but it has to be computed differently. The pseudoinverse of a matrix $\mathbf{B}$ can be defined as the limit

$$\mathbf{B}^{+} = \lim_{\delta \to 0} \bigl(\mathbf{B}^T\mathbf{B} + \delta^2 \mathbf{I}\bigr)^{-1} \mathbf{B}^T.$$

Alternatively, it can be defined using the conditions of Penrose (see Albert [1982]), which state that the matrix $\mathbf{B}^{+}$ is the pseudoinverse of the matrix $\mathbf{B}$ if and only if

- $\mathbf{B}\,\mathbf{B}^{+}$ and $\mathbf{B}^{+}\mathbf{B}$ are symmetric,
- $\mathbf{B}^{+}\mathbf{B}\,\mathbf{B}^{+} = \mathbf{B}$,
- $\mathbf{B}\,\mathbf{B}^{+}\mathbf{B} = \mathbf{B}^{+}$.

The pseudoinverse can also be found using spectral decomposition. The eigenvectors of the pseudoinverse are the same as those of the original matrix, while the corresponding nonzero eigenvalues are the inverses of the nonzero eigenvalues of the original matrix.

A.5 Lagrange Multipliers

The method of Lagrange multipliers provides powerful techniques for solving extremal problems with constraints. We first consider the case of a single constraint equation, then generalize to several constraints.

A.5.1 One Constraint

Suppose we want to find an extremum of a function $f(x, y)$ subject to the constraint $g(x, y) = 0$. If we can solve the latter equation for y,

$$y = \phi(x),$$

we can eliminate y by substitution and find the extrema of

$$f\bigl(x, \phi(x)\bigr)$$

by differentiating with respect to x. Using the chain rule for differentiation, we obtain

$$\frac{\partial f}{\partial x} + \frac{\partial f}{\partial y}\frac{d\phi}{dx} = 0.$$

Often, however, it is impossible or impractical to find a closed-form solution for y in terms of x. In this situation we use the method of Lagrange multipliers. We shall not prove that the method provides necessary conditions for extrema, just indicate why it works.

Consider the curve defined by $g(x, y) = 0$. Let s be a parameter that varies as we move along the curve. Then

$$\frac{\partial g}{\partial x}\frac{dx}{ds} + \frac{\partial g}{\partial y}\frac{dy}{ds} = 0,$$

and the slope of this curve is

$$\frac{dy}{dx} = -\frac{\partial g}{\partial x} \Bigg/ \frac{\partial g}{\partial y} .$$

Substituting this for $d\phi/dx$ in the equation for the extrema derived earlier, we obtain

$$\frac{\partial f}{\partial x}\frac{\partial g}{\partial y} = \frac{\partial f}{\partial y}\frac{\partial g}{\partial x}.$$

This equation applies even when the constraint equation $g(x, y) = 0$ cannot be solved explicitly for y.

Now consider instead the extrema of the function

$$F(x, y, \lambda) \equiv f(x, y) + \lambda g(x, y).$$

Differentiating with respect to x, y, and λ, we have

$$\frac{\partial f}{\partial x} + \lambda\frac{\partial g}{\partial x} = 0 \quad \text{and} \quad \frac{\partial f}{\partial y} + \lambda\frac{\partial g}{\partial y} = 0.$$

If we eliminate λ, we obtain again

$$\frac{\partial f}{\partial x}\frac{\partial g}{\partial y} = \frac{\partial f}{\partial y}\frac{\partial g}{\partial x}.$$

Thus the extrema of $f(x, y)$ subject to the constraint $g(x, y) = 0$ can be found by finding the extrema of $F(x, y, \lambda)$.

To make this seem plausible, consider moving along the curve defined by $g(x, y) = 0$, searching for an extremum of $f(x, y)$. There can be no extremum where the contours of constant $f(x, y)$ cross the curve we are following, since we can move a small distance along the curve and find a slightly larger or slightly smaller value of $f(x, y)$, as needed. The extrema are where the contours of constant $f(x, y)$ are parallel to the constraint curve. Note also that the constraint curve in turn is a curve of constant

$g(x,y)$. Contours of constant $f(x,y)$ are perpendicular to the gradient of $f(x,y)$,

$$\nabla f = \left(\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}\right)^T,$$

while contours of constant $g(x,y)$ are perpendicular to the gradient of $g(x,y)$,

$$\nabla g = \left(\frac{\partial g}{\partial x}, \frac{\partial g}{\partial y}\right)^T.$$

These two gradients must be parallel.

Consider now finding an extremum of $F(x,y,\lambda)$. Differentiation gives us

$$\frac{\partial f}{\partial x} + \lambda\frac{\partial g}{\partial x} = 0 \quad \text{and} \quad \frac{\partial f}{\partial y} + \lambda\frac{\partial g}{\partial y} = 0,$$

or

$$\left(\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}\right)^T = -\lambda\left(\frac{\partial g}{\partial x}, \frac{\partial g}{\partial y}\right)^T,$$

which is a statement of the condition that the two gradients must be parallel. The factor $-\lambda$ is simply the ratio of the magnitudes of the two gradients.

As an example, let us find the point on the line

$$x\sin\theta - y\cos\theta + \rho = 0$$

that is closest to the origin. Here we have to minimize $x^2 + y^2$ subject to the given constraint. Conversely, we can minimize

$$(x^2 + y^2) + \lambda(x\sin\theta - y\cos\theta + \rho).$$

Differentiating with respect to x and y, we find

$$2x + \lambda\sin\theta = 0 \qquad \text{and} \qquad 2y - \lambda\cos\theta = 0.$$

Thus $x\cos\theta + y\sin\theta = 0$. Substituting in the constraint equation, we obtain

$$x\sin\theta + x\cos^2\theta/\sin\theta + \rho = 0, \qquad \text{or} \qquad x = -\rho\sin\theta,$$

and

$$-y\sin^2\theta/\cos\theta - y\cos\theta + \rho = 0, \qquad \text{or} \qquad y = +\rho\cos\theta.$$

The same method applies if we have more than three independent variables. To find an extremum of $f(x,y,z)$ subject to the constraint

$g(x, y, z) = 0$, we look for places where the surfaces of constant $f(x, y, z)$ are tangent to the surfaces of constant $g(x, y, z)$. Because the gradient is perpendicular to the tangent plane, we can also look for places where the gradient of $f(x, y, z)$ is parallel to the gradient of $g(x, y, z)$. We thus look for extrema of

$$f(x, y, z) + \lambda g(x, y, z),$$

since this leads to the equations

$$\frac{\partial f}{\partial x} + \lambda \frac{\partial g}{\partial x} = 0,$$
$$\frac{\partial f}{\partial y} + \lambda \frac{\partial g}{\partial y} = 0,$$
$$\frac{\partial f}{\partial z} + \lambda \frac{\partial g}{\partial z} = 0,$$

or

$$\left(\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z} \right)^T = -\lambda \left(\frac{\partial g}{\partial x}, \frac{\partial g}{\partial y}, \frac{\partial g}{\partial z} \right)^T .$$

A.5.2 More than One Constraint

With three independent variables, we can add a second constraint. The extrema of $f(x, y, z) = 0$ subject to the constraints $g(x, y, z) = 0$ and $h(x, y, z) = 0$ are the same as the extrema of

$$f(x, y, z) + \lambda g(x, y, z) + \mu h(x, y, z)$$

subject to those constraints. Differentiating with respect to x, y, and z yields

$$\frac{\partial f}{\partial x} + \lambda \frac{\partial g}{\partial x} + \mu \frac{\partial h}{\partial x} = 0,$$
$$\frac{\partial f}{\partial y} + \lambda \frac{\partial g}{\partial y} + \mu \frac{\partial h}{\partial y} = 0,$$
$$\frac{\partial f}{\partial z} + \lambda \frac{\partial g}{\partial z} + \mu \frac{\partial h}{\partial z} = 0.$$

These equations state that the gradient of f must be a linear combination of the gradients of g and h:

$$\nabla f = -\lambda \nabla g - \mu \nabla h.$$

The constraints $g(x, y, z) = 0$ and $h(x, y, z) = 0$ each define a surface. Their intersection is the curve along which we search for extrema. The gradient of a surface is perpendicular to the tangent plane. Thus curves on a surface are perpendicular to the gradient. In particular, the intersection of the two surfaces is perpendicular to both gradients. The curve of intersection is thus parallel to the cross-product of the two gradients. At an extremum, the gradient of $f(x, y, z)$ should not have any component in this direction—otherwise we can increase or decrease the value of $f(x, y, z)$ by moving a little along the curve. The gradient of $f(x, y, z)$ will satisfy this condition if and only if it can be expressed as a linear combination of the gradients of $g(x, y, z)$ and $h(x, y, z)$.

As an example, let us find the box with largest volume subject to the constraints that one face of the box has unit area and that the sum of the width, height, and depth of the box is four. Let the dimensions of the box be a, b, and c. We minimize

$$abc + \lambda(ab - 1) + \mu(a + b + c - 4).$$

Differentiating with respect to a, b, and c yields

$$\begin{aligned} bc + \lambda b + \mu &= 0, \\ ac + \lambda a + \mu &= 0, \\ ab + \mu &= 0. \end{aligned}$$

Eliminating λ and μ from these equations, we obtain $a = b$. From the first constraint it follows that $a = b = 1$. The second constraint gives $c = 2$.

A.5.3 The General Case

Let $\mathbf{x} = (x_1, x_2, \ldots, x_n)^T$ be a vector in an n-dimensional space. The set of values $\mathbf{x}$ that satisfy the constraint $g(\mathbf{x}) = 0$ form a subspace. Consider some curve lying entirely in this subspace. Let s be a parameter that varies as we move along this curve. The direction of the curve at a point is defined by the tangent at that point,

$$\frac{d\mathbf{x}}{ds} = \left(\frac{dx_1}{ds}, \frac{dx_2}{ds}, \ldots, \frac{dx_n}{ds} \right)^T .$$

The rate of change of $g(\mathbf{x})$ with s is given by

$$\frac{dg}{ds} = \frac{\partial g}{\partial x_1}\frac{dx_1}{ds} + \frac{\partial g}{\partial x_2}\frac{dx_2}{ds} + \cdots + \frac{\partial g}{\partial x_n}\frac{dx_n}{ds} = \nabla g \cdot \frac{d\mathbf{x}}{ds},$$

where ∇g is the gradient of g,

$$\nabla g = \left(\frac{\partial g}{\partial x_1}, \frac{\partial g}{\partial x_2}, \ldots, \frac{\partial g}{\partial x_n} \right)^T .$$

Because the curve remains in the subspace where $g(\mathbf{x}) = 0$, we have

$$\nabla g \cdot \frac{d\mathbf{x}}{ds} = 0.$$

That is, the curve must at each point be perpendicular to the gradient of $g(\mathbf{x})$. The allowed tangent directions at a particular point form an $(n-1)$-dimensional subspace as long as the gradient is nonzero. We can see this by noting that only $n-1$ components of the tangent vector are independent, the remaining component being constrained by the last equation.

Now suppose that there are m constraints $g_i(\mathbf{x}) = 0$ for $i = 1, 2, \ldots, m$. The intersection of the subspaces defined by each of the constraints individually is also a subspace. A curve lying in this common subspace must be perpendicular to all of the gradients of the g_i; thus

$$\nabla g_i \cdot \frac{d\mathbf{x}}{ds} = 0 \qquad \text{for } i = 1, 2, \ldots, m.$$

If the m gradients are linearly independent, the common subspace has dimension $n-m$, since only $n-m$ components of the tangent vector can be freely chosen, the rest being constrained by the m equations above.

If $f(\mathbf{x})$ is to have an extremum at a point in the subspace defined by the constraints, then the first derivative of f along any curve lying in the subspace must be zero. Now

$$\frac{df}{ds} = \nabla f \cdot \frac{d\mathbf{x}}{ds},$$

so that we want

$$\nabla f \cdot \frac{d\mathbf{x}}{ds} = 0$$

for any tangent direction that satisfies

$$\nabla g_i \cdot \frac{d\mathbf{x}}{ds} = 0 \qquad \text{for } i = 1, 2, \ldots, m.$$

That is, at the extremum, the tangent must be perpendicular to the gradient of f as well. This certainly is the case if the gradient of f happens to be a linear combination of the gradients of the g_i at the point. What we want to show is that ∇f must be a linear combination of the ∇g_i at an extremum.

It is easy to show that the constraints

$$\nabla g_i \cdot \frac{d\mathbf{x}}{ds} = 0$$

define a vector space. Any vector can be uniquely decomposed into a component that lies in this subspace and one that is orthogonal to it.

The vector ∇f can be decomposed into a component $\mathbf{g}$ that is a linear combination of the ∇g_i and a component $\mathbf{c}$ that is orthogonal to each of the ∇g_i. Suppose that $\mathbf{c}$ is nonzero. Then

$$\nabla f \cdot \frac{d\mathbf{x}}{ds} = \mathbf{g} \cdot \frac{d\mathbf{x}}{ds} + \mathbf{c} \cdot \frac{d\mathbf{x}}{ds} = \mathbf{c} \cdot \frac{d\mathbf{x}}{ds},$$

since $\mathbf{g}$ is a linear combination of the ∇g_i. We can choose a curve for which

$$\frac{d\mathbf{x}}{ds} = \mathbf{c},$$

since $\nabla g_i \cdot \mathbf{c} = 0$ for $i = 1, 2, \ldots, m$. In this case

$$\nabla f \cdot \frac{d\mathbf{x}}{ds} = \mathbf{c} \cdot \mathbf{c} \neq 0.$$

This contradicts the condition for an extremum, and $\mathbf{c}$ must therefore be zero after all. That is, ∇f must be a linear combination of the gradients ∇g_i. We can write this condition as

$$\nabla f = -\sum_{i=1}^{m} \lambda_i \nabla g_i$$

for some set of coefficients λ_i.

Consider now the function

$$f(\mathbf{x}) + \sum_{i=1}^{m} \lambda_i g_i(\mathbf{x}).$$

If we try to find an extremum by differentiating with respect to $\mathbf{x}$, we obtain

$$\nabla f + \sum_{i=1}^{m} \lambda_i \nabla g_i = \mathbf{0},$$

which is just the equation shown to be satisfied at an extremum of f.

To summarize, then, the extrema of $f(\mathbf{x})$, subject to the m constraints $g_i(\mathbf{x}) = 0$, can be found by locating the extrema of

$$f(\mathbf{x}) + \sum_{i=1}^{m} \lambda_i g_i(\mathbf{x})$$

subject to the same constraints. Here $\mathbf{x}$ is a vector with n components and $n > m$.

A.6 The Calculus of Variations

Calculus teaches us how to find extrema of functions. We are allowed to vary one or more parameters of some function. A solution is a set of parameters that corresponds to an extremum of the function. Differentiation of the function leads to a set of (algebraic) equations that represent necessary conditions for an extremum.

In the calculus of variations we look for extrema of expressions that depend on functions rather than parameters. Such expressions are called *functionals*. Now we obtain differential equations rather than ordinary equations to represent the necessary conditions for an extremum.

A.6.1 Problems without Constraints

As an example, consider the simple integral

$$I = \int_{x_1}^{x_2} F(x, f, f')\, dx.$$

Here F depends on the unknown function f and its derivative f'. Let us assume that the curve to be found must pass through the points $f(x_1) = f_1$ and $f(x_2) = f_2$. Suppose that the function $f(x)$ is a solution of the extremum problem. Then we expect that small variations in $f(x)$ should not change the integral significantly.

Let $\eta(x)$ be a test function. If we add $\epsilon\,\eta(x)$ to $f(x)$, we expect that the integral will change by an amount proportional to ϵ^2 for small values of ϵ. If, instead, it varied linearly with ϵ, we could increase or decrease the integral as desired and would therefore not be at an extremum. To be precise, we want

$$\left.\frac{dI}{d\epsilon}\right|_{\epsilon=0} = 0.$$

This must be true for all test functions $\eta(x)$.

In our specific problem, we must have $\eta(x_1) = 0$ and $\eta(x_2) = 0$ to satisfy the boundary conditions. Also, if $f(x)$ is replaced by $f(x) + \epsilon\,\eta(x)$, then $f'(x)$ is replaced by $f'(x) + \epsilon\,\eta'(x)$. The integral then becomes

$$I = \int_{x_1}^{x_2} F(x, f + \epsilon\eta, f' + \epsilon\eta')\, dx.$$

If F is suitably differentiable, we can expand the integrand in a Taylor series,

$$F(x, f+\epsilon\eta, f'+\epsilon\eta') \\ = F(x,f,f') + \epsilon\frac{\partial}{\partial f}F(x,f,f')\eta(x) + \epsilon\frac{\partial}{\partial f'}F(x,f,f')\eta'(x) + e,$$

where e consists of terms in higher powers of ϵ. Thus

$$I = \int_{x_1}^{x_2} \big(F + \epsilon\eta(x)F_f + \epsilon\eta' F_{f'} + e\big)\,dx,$$

and differentiating with respect to ϵ and setting ϵ equal to zero yields

$$0 = \int_{x_1}^{x_2} \big(\eta(x)F_f + \eta'(x)F_{f'}\big)\,dx.$$

Using integration by parts, we see that

$$\int_{x_1}^{x_2} \eta'(x)F_{f'}\,dx = [\eta(x)F_{f'}]_{x_1}^{x_2} - \int_{x_1}^{x_2} \eta(x)\frac{d}{dx}F_{f'}\,dx,$$

where the first term is zero because of the boundary conditions. We must therefore have

$$0 = \int_{x_1}^{x_2} \eta(x)\left(F_f - \frac{d}{dx}F_{f'}\right)\,dx.$$

If this is to be true for all test functions $\eta(x)$, then

$$F_f - \frac{d}{dx}F_{f'} = 0.$$

This is called the *Euler equation* for this problem.

The method can be generalized in a number of ways. First, suppose that the boundary conditions $f(x_1) = f_1$ and $f(x_2) = f_2$ are not given. Then in order for the term

$$[\eta(x)F_{f'}]_{x_1}^{x_2}$$

to be zero for all possible test functions $\eta(x)$, we must introduce the *natural boundary conditions*

$$F_{f'} = 0 \qquad \text{at } x = x_1 \text{ and } x = x_2.$$

Next, the integrand might contain higher derivatives,

$$I = \int_{x_1}^{x_2} F(x, f, f', f'', \dots)\,dx.$$

The Euler equation in this case becomes

$$F_f - \frac{d}{dx}F_{f'} + \frac{d^2}{dx^2}F_{f''} - \cdots = 0.$$

In this case we must specify the boundary values of all but the highest derivatives in order to pose the problem properly.

We can also treat the case in which the integrand depends on several functions $f_1(x)$, $f_2(x)$, ... instead of just one. That is,

$$I = \int_{x_1}^{x_2} F(x, f_1, f_2, \ldots, f_1', f_2', \ldots)\, dx.$$

In this case there are as many Euler equations as there are unknown functions:

$$F_{f_i} - \frac{d}{dx}F_{f_i'} = 0.$$

Consider next a case in which there are two independent variables x and y and we are to find a function $f(x, y)$ that yields an extremum of the integral

$$I = \iint_D F(x, y, f, f_x, f_y)\, dx\, dy.$$

Here f_x and f_y are the partial derivatives of f with respect to x and y, respectively, and the integral is over some simply-connected closed region D. We introduce a test function $\eta(x, y)$ and add $\epsilon\,\eta(x, y)$ to $f(x, y)$. We are given the values of $f(x, y)$ on the boundary ∂D of the region, so the test function must be zero on the boundary. Taylor series expansion yields

$$\begin{aligned}
&F(x, y, f + \epsilon\eta, f_x + \epsilon\eta_x, f_y + \epsilon\eta_y) \\
&\quad = F(x, y, f, f_x, f_y) + \epsilon\frac{\partial}{\partial f}F(x, y, f, f_x, f_y)\eta(x, y) \\
&\qquad + \epsilon\frac{\partial}{\partial f_x}F(x, y, f, f_x, f_y)\eta_x(x, y) + \epsilon\frac{\partial}{\partial f_y}F(x, y, f, f_x, f_y)\eta_y(x, y) + e,
\end{aligned}$$

where e consists of terms in higher powers of ϵ. Thus

$$I = \iint_D \left(F + \epsilon\eta F_f + \epsilon\eta_x F_{f_x} + \epsilon\eta_y F_{f_y}\right) dx\, dy,$$

and differentiating with respect to ϵ and setting ϵ equal to zero yields

$$0 = \iint_D \left(\eta F_f + \eta_x F_{f_x} + \eta_y F_{f_y}\right) dx\, dy.$$

Now by Gauss's integral theorem,

$$\iint_D \left(\frac{\partial Q}{\partial x} + \frac{\partial P}{\partial y} \right) dx\, dy = \int_{\partial D} \big(Q\, dy - P\, dx \big),$$

so that

$$\iint_D \left(\frac{\partial}{\partial x}(\eta F_{f_x}) + \frac{\partial}{\partial y}(\eta F_{f_y}) \right) dx\, dy = \int_{\partial D} \big(\eta F_{f_x}\, dy - \eta F_{f_y}\, dx \big).$$

Given the boundary conditions, the term on the right must be zero, so that

$$\iint_D \big(\eta_x F_{f_x} + \eta_y F_{f_y} \big)\, dx\, dy = - \iint_D \left(\eta \frac{\partial}{\partial x} F_{f_x} + \eta \frac{\partial}{\partial y} F_{f_y} \right) dx\, dy.$$

Consequently,

$$0 = \iint_D \eta \left(F_f - \frac{\partial}{\partial x} F_{f_x} - \frac{\partial}{\partial y} F_{f_y} \right) dx\, dy$$

for all test functions η. We must have, then, that

$$F_f - \frac{\partial}{\partial x} F_{f_x} - \frac{\partial}{\partial y} F_{f_y} = 0.$$

Here the Euler equation is a partial differential equation. An immediate extension is to the case in which the value of f on the boundary ∂D is not specified. For the integral

$$\int_{\partial D} \eta \big(F_{f_x} dy - F_{f_y} dx \big)$$

to be zero for all test functions η, we must have

$$F_{f_x} \frac{dy}{ds} = F_{f_y} \frac{dx}{ds},$$

where s is a parameter that varies along the boundary.

The extension to more than two independent variables is also immediate.

A.6.2 Variational Problems with Constraints

A problem in the calculus of variations can also have constraints. Suppose, for example, that we want to find an extremum of

$$I = \int_{x_1}^{x_2} F(x, f_1, f_2, \ldots, f_n, f_1', f_2', \ldots, f_n')\, dx$$

subject to the constraints $g_i(x, f_1, f_2, \ldots, f_n) = 0$ for $i = 1, 2, \ldots, m$, with $m < n$. We can solve the modified Euler equations

$$\frac{\partial \Phi}{\partial f_i} - \frac{d}{dx}\frac{\partial \Phi}{\partial f_i'} = 0 \qquad \text{for } i = 1, 2, \ldots, n$$

subject to the constraints. Here

$$\Phi \equiv F + \sum_{i=1}^{m} \lambda_i(x) g_i(x, f_1, f_2, \ldots, f_n).$$

The unknown functions $\lambda_i(x)$ are again called *Lagrange multipliers.*

Constraints in the form of integrals are treated similarly. Suppose we want to find an extremum of the integral

$$I = \int_{x_1}^{x_2} F(x, f_1, f_2, \ldots, f_n, f_1', f_2', \ldots, f_n')\, dx$$

subject to the constraints

$$\int_{x_1}^{x_2} g_i(x, f, f_1, f_2, \ldots, f_n, f_1', f_2', \ldots, f_n')\, dx = c_i \qquad \text{for } i = 1, 2, \ldots, m,$$

where the c_i are given constants. We now solve the modified Euler equations

$$\frac{\partial \Psi}{\partial f_i} - \frac{d}{dx}\frac{\partial \Psi}{\partial f_i'} = 0 \qquad \text{for } i = 1, 2, \ldots, m$$

subject to the constraints. Here

$$\Psi \equiv F + \sum_{i=1}^{m} \lambda_i g_i(x, f_1, f_2, \ldots, f_n).$$

The unknown constants λ_i are still called *Lagrange multipliers.*

A.7 References

A valuable mathematical encyclopedia is the *Mathematical Handbook for Engineers and Scientists* by Korn & Korn [1968]. Difficult integrals can be looked up in the *Table of Integrals, Series, and Products* by Gradshteyn & Ryzhik [1980]. All elementary and many special functions can be found in the *Handbook of Mathematical Functions with Formulas, Graphs, and Mathematical Tables* edited by Abramowitz & Stegan [1964]. Smaller collections of this kind of information may be found in Burington's *Handbook* *of Mathematical Tables and Formulas* [1973] and Dwight's *Tables of Integrals and Other Mathematical Data* [1964].

Chisholm provides an elementary treatment of vectors in *Vectors in Three-Dimensional Space* [1978], while Schey deals with differential operators applied to vectors in *Div, Grad, Curl, and All That: An Informal Text on Vector Calculus* [1973]. Generally useful mathematical tools are covered in many books, such as Hildebrand's *Methods of Applied Mathematics* [1952].

There is no shortage of books on probability and statistics. One such is Drake's *Fundamentals of Applied Probability Theory* [1967].

The calculus of variations is explained in *Methods of Mathematical Physics*, volume I, by Courant & Hilbert [1953] and *Calculus of Variations: With Applications to Physics & Engineering* by Weinstock [1974].

Least-squares methods often lead to problems that can be tackled using the pseudoinverse. Here one can recommend Albert's *Regression and the Moore–Penrose Pseudoinverse* [1972]. Gill, Murray, & Wright cover practical aspects of optimization problems in *Practical Optimization* [1981]. Deeper coverage of the theoretical issues can be found in Luenberger's *Introduction to Linear and Nonlinear Programming* [1973].

Numerical methods are covered in such books as *Elementary Numerical Analysis—an Algorithmic Approach* by Conte & de Boor [1972] and Hamming's *Numerical Methods for Scientists and Engineers* [1962].