19.7: Appendix - Aspects of Multivariate Calculus

Multivariate calculus provides the framework for handling systems having many variables associated with each of several bodies. It is assumed that the reader has studied linear differential equations plus multivariate calculus and thus has been exposed to the calculus used in classical mechanics. Chapter 5 of this book introduced variational calculus which covers several important aspects of multivariate calculus such as Euler's variational calculus and Lagrange multipliers. This appendix provides a brief review of a selection of other aspects of multivariate calculus that feature prominently in classical mechanics.

Partial Differentiation

The extension of the derivative to multivariate calculus involves use of partial derivatives. The partial derivative with respect to the variable x_i of a multivariate function $f(x_1, x_2, \ldots, x_N)$ involves taking the normal one-variable derivative with respect to x_i assuming that the other $N-1$ variables are held constant. That is,

$$\frac{\partial f\left(x_1, x_2, \ldots x_N\right)}{\partial x_i}=\lim_{h_i \rightarrow 0}\left[\frac{f\left(x_1, x_2, \ldots x_{i-1},\left(x_i+h_i\right), \ldots x_N\right)-f\left(x_1, x_2, \ldots, x_N\right)}{h_i}\right] \tag{19.7.1}$$

where it will be assumed that the function $f(x)$ is a continuously-differentiable function to n^{th} order, then all partial derivatives of that order or less are independent of the order in which they are performed. That is,

$$\frac{\partial^2 f(x)}{\partial x_i \partial x_j}=\frac{\partial^2 f(x)}{\partial x_j \partial x_i} \tag{19.7.2}$$

The chain rule for partial differentiation gives that

$$\frac{\partial f(y_1, y_2, \ldots, y_N)}{\partial y_j}=\sum_{k=1}^N \frac{\partial f(x)}{\partial x_k} \frac{\partial x_k(y)}{\partial y_j} \tag{19.7.3}$$

The total differential of a multivariate function $f(x)$ is

$$df=\sum_{k=1}^N \frac{\partial f(x)}{\partial x_k} dx_k \tag{19.7.4}$$

This can be extended to higher-order derivatives using the operator formalism

$$d^n f(x)=\left(dx_1 \frac{\partial}{\partial x_1}+\ldots+dx_N \frac{\partial}{\partial x_N}\right)^n f(x)=\sum dx_{j_1} \ldots dx_{j_n} \frac{\partial^n f(x)}{\partial x_{j_1} \ldots \partial x_{j_n}} \tag{19.7.5}$$

Linear Operators

The linear operator notation provides a powerful, elegant, and compact way to express, and apply, the equations of multivariate calculus; it is used extensively in mathematics and physics. The linear operators typically comprise partial derivatives that act on scalar, vector, or tensor fields. Table 19.7.1 lists a few elementary examples of the use of linear operators in this textbook. The first four linear operators involve the widely used del operator $\boldsymbol{\nabla}$ to generate the gradient, divergence and curl as described in appendices 19.7 and 19.8. The fifth and sixth linear operators act on the Lagrangian in Lagrangian mechanics applications. The final two linear operators act on the wavefunction for wave mechanics.

Table 19.7.1: Examples of linear operators used in this textbook.

Name	Partial derivative	Field	Action
Gradient	$\boldsymbol{\nabla} \equiv \hat{i}\frac{\partial}{\partial x}+\hat{j}\frac{\partial}{\partial y}+\hat{\mathbf{k}}\frac{\partial}{\partial z}$	Scalar potential V	$\mathbf{E}=\boldsymbol{\nabla} V$
Divergence	$\boldsymbol{\nabla}\cdot \equiv\left(\hat{i}\frac{\partial}{\partial x}+\hat{j}\frac{\partial}{\partial y}+\hat{\mathbf{k}}\frac{\partial}{\partial z}\right)\cdot$	Vector field $\mathbf{E}$	$\boldsymbol{\nabla}\cdot\mathbf{E}$
Curl	$\boldsymbol{\nabla}\times \equiv\left(\hat{i}\frac{\partial}{\partial x}+\hat{j}\frac{\partial}{\partial y}+\hat{\mathbf{k}}\frac{\partial}{\partial z}\right)\times$	Vector field $\mathbf{E}$	$\boldsymbol{\nabla}\times\mathbf{E}$

Name	Partial derivative	Field	Action
Laplacian	$\nabla^2 = \boldsymbol{\nabla} \cdot \boldsymbol{\nabla} \equiv \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$	Scalar potential V	$\nabla^2 V$
Euler-Lagrange	$\Lambda_j \equiv \frac{d}{dt}\frac{\partial}{\partial \dot{q}_j} - \frac{\partial}{\partial q_j}$	Scalar Lagrangian L	$\Lambda L = 0$
Canonical momentum	$p_j \equiv \frac{\partial}{\partial \dot{q}_j}$	Scalar Lagrangian L	$p_j \equiv \frac{\partial L}{\partial \dot{q}_j}$
Canonical momentum	$p_j \equiv \frac{\hbar}{i}\frac{\partial}{\partial \dot{q}_j}$	Wavefunction Ψ	$p_j \Psi \equiv \frac{\hbar}{i}\frac{\partial \Psi}{\partial \dot{q}_j}$
Hamiltonian	$H = i\hbar\frac{\partial}{\partial t}$	Wavefunction Ψ	$H\Psi = i\hbar\frac{\partial \Psi}{\partial t} = E\Psi$

There are three ways of expressing operations such as addition, multiplication, transposition or inversion of operations that are completely equivalent because they all are based on the same principles of linear algebra. For example, a transformation $\mathbf{O}$ acting on a vector $\mathbf{A}$ can produce the vector $\mathbf{B}$. The simplest way to express this transformation is in terms of components

$$B_i = \sum_{j=1}^{3} O_{ij} A_j \tag{19.7.6}$$

Another way is to use matrix mechanics where the 3×3 matrix $(\mathbf{O})$ transforms the column vector $(\mathbf{A})$ to the column vector $(\mathbf{B})$, that is,

$$(\mathbf{B}) = (\mathbf{O})(\mathbf{A}) \tag{19.7.7}$$

The third approach is to assume an operator $\mathbf{O}$ acts on the vector $\mathbf{A}$

$$\mathbf{B} = \mathbf{OA} \tag{19.7.8}$$

In classical mechanics, and quantum mechanics, these three equivalent approaches are used and exploited extensively and interchangeably. In particular the rules of matrix manipulation, that are given in appendix 19.1, are synonymous, and equivalent to, those that apply for operator manipulation. If the operator is complex then the operator properties are summarized as follows.

The generalization of the transpose for complex operators is the *Hermitian conjugate* $O^\dagger$

$$O^\dagger_{ij} = O^*_{ji} \tag{19.7.9}$$

Note also that

$$\mathbf{O}^\dagger = (O^*)^T = (O^T)^* \tag{19.7.10}$$

The generalization of a symmetric matrix is *Hermitian*, that is, O is equal to its Hermitian conjugate

$$O^\dagger_{ij} = O^*_{ji} = O_{ij} \tag{19.7.11}$$

For a real matrix the complex conjugation has no effect so the matrix is real and symmetric.

The generalization of orthogonal is *unitary* for which the operator is unitary if it is non-singular and

$$O^{-1} = O^\dagger \tag{19.7.12}$$

which implies

$$OO^\dagger = U = O^\dagger O \tag{19.7.13}$$

Transformation Jacobian

The Jacobian determinant, which is usually called the Jacobian, is used extensively in mechanics for both rotational and translational coordinate transformations. The Jacobian determinant is defined as being the ratio of the n-dimensional volume element $dx_1dx_2\dots dx_n$ in one coordinate system, to the volume element $dy_1dy_2\dots dy_n$ in the second coordinate system. That is

$$J(y_1y_2\dots y_n) \equiv \frac{\partial x_1 \partial x_2 \dots \partial x_n}{\partial y_1 \partial y_2 \dots \partial y_n} = \begin{vmatrix} \frac{\partial x_1}{\partial y_1} & \frac{\partial x_1}{\partial y_2} & \dots & \frac{\partial x_1}{\partial y_n} \\ \frac{\partial x_2}{\partial y_1} & \frac{\partial x_2}{\partial y_2} & \dots & \frac{\partial x_2}{\partial y_n} \\ \vdots & \vdots & \vdots & \vdots \\ \frac{\partial x_n}{\partial y_1} & \frac{\partial x_n}{\partial y_2} & \dots & \frac{\partial x_n}{\partial y_n} \end{vmatrix} \tag{19.7.14}$$

Transformation of integrals

Consider a coordinate transformation for the integral of the function $f(x_1, x_2, ..x_n)$ to the integral of a function $g(y_1, y_2, \dots y_n)$ where $y_i = h(x_1, x_2, \dots x_n)$. The coordinate transformation of the integral equation can be expressed in terms of the Jacobian $J(y_1y_2\dots y_n)$

$$\int f(x_1, x_2, \dots x_n)\, dx_1dx_2\dots dx_n = \int g(y_1, y_2, \dots y_n)\, dy_1dy_2\dots dy_n = \tag{19.7.15}$$

$$\int f(x_1, x_2, \dots x_n) \frac{\partial x_1 \partial x_2 \dots \partial x_n}{\partial y_1 \partial y_2 \dots \partial y_n} dy_1dy_2\dots dy_n = \int f(y_1, y_2, ..y_n)\, J(y_1, y_2, \dots y_n)\, dy_1dy_2\dots dy_n$$

Transformation of differential equations

The differential cross sections for scattering can be defined either by the number of a definite kind of particle/per event, going into the volume element in momentum space $dp_1dp_2dp_3$, or by the number going into the solid angle element having momentum between p and $p + dp$. That is, the first definition can be written as a differential equation

$$\frac{\partial^3 S(p_1, p_2, p_3)}{\partial p_1 \partial p_2 \partial p_3} dp_1dp_2dp_3 = \frac{\partial^3 S(p_1(p\theta\phi), p_2(p\theta\phi), p_3(p\theta\phi))}{\partial p_1 \partial p_2 \partial p_3} \frac{\partial(p_1, p_2, p_3)}{\partial(p, \theta, \phi)} dpd\theta d\phi \tag{19.7.16}$$

As shown in table 19.3.4, $dp_1dp_2dp_3 = p^2 \sin\theta dpd\theta d\phi$, that is, the Jacobian equals $p^2 \sin\theta$. Thus Equation 19.7.16 can be written as

$$\frac{\partial^3 S(p_1, p_2, p_3)}{\partial p_1 \partial p_2 \partial p_3} dp_1dp_2dp_3 = \left[\frac{\partial^3 S}{\partial p_1 \partial p_2 \partial p_3} p^2\right] (\sin\theta dpd\theta d\phi) = \frac{\partial^2 \sigma(p, \theta, \phi)}{\partial p \partial \Omega} dpd\Omega \tag{19.7.17}$$

The differential cross section is defined by

$$\frac{\partial^2 \sigma(p, \theta, \phi)}{\partial p \partial \Omega} \equiv \frac{\partial^3 S}{\partial p_1 \partial p_2 \partial p_3} p^2 \tag{19.7.18}$$

where the p^2 factor is absorbed into the cross section and the solid angle term is factored out

Properties of the Jacobian

In classical mechanics the Jacobian often is extended from 3 dimensions to n-dimensional transformations. The Jacobian is unity for unitary transformations such as rotations and linear translations which implies that the volume element is preserved. It will be shown that this also is true for a certain class of transformations in classical mechanics that are called canonical transformations. The Jacobian transforms the local density to be correct for any scale transformations such as transforming linear dimensions from centimeters to inches.

Example 19.7.1: Jacobian for transform from cartesian to spherical coordinates

Consider the transform in the three-dimensional integral $\int(x_1, x_2, x_3)dx_1dx_2dx_3$ under transformation from cartesian coordinates (x_1, x_2, x_3) to spherical coordinates (r, θ, ϕ). The transformation is governed by the geometric relations $x_1 = r\sin\theta\cos\phi, x_2 = r\sin\theta\sin\phi, x_3 = r\cos\theta$. For this transformation the Jacobian determinant equals

$$J(r, \theta, \phi) = \begin{vmatrix} \sin\theta\cos\phi & r\cos\theta\cos\phi & -r\sin\theta\sin\phi \\ \sin\theta\sin\phi & r\cos\theta\sin\phi & r\sin\theta\cos\phi \\ \cos\theta & -r\sin\theta & 0 \end{vmatrix} = r^2 \sin\theta$$

Thus the three-dimensional volume integral transforms to

$$\int f(x_1,x_2,x_3)dx_1dx_2dx_3 = \int f(r,\theta,\phi)J(r,\theta,\phi)drd\theta d\phi = \int f(r,\theta,\phi)r^2\sin\theta drd\theta d\phi$$

which is the well-known volume integral in spherical coordinates.

Legendre transformation

Hamiltonian mechanics can be derived directly from Lagrange mechanics by considering the Legendre transformation between the conjugate variables $(\mathbf{q},\dot{\mathbf{q}},t)$ and $(\mathbf{q},\mathbf{p},t)$. Such a derivation is of considerable importance in that it shows that Hamiltonian mechanics is based on the same variational principles as those used to derive Lagrangian mechanics; that is d'Alembert's Principle or Hamilton's Principle. The general problem of converting Lagrange's equations into the Hamiltonian form hinges on the inversion of equation $(8.1.3)$ that defines the generalized momentum $\mathbf{p}$. This inversion is simplified by the fact that $(8.1.3)$ is the first partial derivative of the Lagrangian $L(\mathbf{q},\dot{\mathbf{q}},t)$ which is a scalar function.

Consider transformations between two functions $F(\mathbf{u},\mathbf{w})$ and $G(\mathbf{v},\mathbf{w})$ where $\mathbf{u}$ and $\mathbf{v}$ are the active variables related by the functional form

$$\mathbf{v} = \boldsymbol{\nabla}_{\mathbf{u}}F(\mathbf{u},\mathbf{w}) \tag{19.7.19}$$

and where $\mathbf{w}$ designates passive variables and $\boldsymbol{\nabla}_{\mathbf{u}}F(\mathbf{u},\mathbf{w})$ is the first-order derivative of $F(\mathbf{u},\mathbf{w})$, i.e. the gradient, with respect to the components of the vector $\mathbf{u}$. The Legendre transform states that the inverse formula can always be written in the form

$$\mathbf{u} = \boldsymbol{\nabla}_{\mathbf{v}}G(\mathbf{v},\mathbf{w}) \tag{19.7.20}$$

where the function $G(\mathbf{v},\mathbf{w})$ is related to $F(\mathbf{u},\mathbf{w})$ by the symmetric relation

$$G(\mathbf{v},\mathbf{w}) + F(\mathbf{u},\mathbf{w}) = \mathbf{u}\cdot\mathbf{v} \tag{19.7.21}$$

and where the scalar product $\mathbf{u}\cdot\mathbf{v} = \sum_{i=1}^{N} u_i v_i$.

Furthermore the derivatives with respect to all the passive variables $\{w_i\}$ are related by

$$\boldsymbol{\nabla}_{\mathbf{w}}F(\mathbf{u},\mathbf{w}) = -\boldsymbol{\nabla}_{\mathbf{w}}G(\mathbf{v},\mathbf{w}) \tag{19.7.22}$$

The relationship between the functions $F(\mathbf{u},\mathbf{w})$ and $G(\mathbf{v},\mathbf{w})$ is symmetrical and each is said to be the Legendre transform of the other.

Exercises

1. Below you will find a set of integrals. Your teaching assistant will divide you into groups and each group will be assigned one integral to work on. Once your group has solved the integral, write the solution on the board in the space provided by the teaching assistant.

(a) $\int_0^{2\pi}\int_0^{\pi/4}\int_0^{\cos\theta} r^2\sin\theta drd\theta d\phi$

(b) $\int(\frac{\dot{\mathbf{r}}}{r} - \frac{\mathbf{r}\dot{r}}{r^2})dt$

(c) $\int_S \mathbf{A}\cdot d\mathbf{a}$ where $\mathbf{A} = x\hat{i} + y\hat{j} + z\hat{\mathbf{k}}$ and S is the sphere $x^2+y^2+z^2=9$.

(d) $\int_S(\boldsymbol{\nabla}\times\mathbf{A})\cdot d\mathbf{a}$ where $\mathbf{A} = y\hat{i} + z\hat{j} + x\hat{\mathbf{k}}$ and S is the surface defined by the paraboloid $z = 1 - x^2 - y^2$, where $z \geq 0$.