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Kwang Soo Cho

Viscoelasticity of Polymers

Theory and Numerical Algorithms

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To my wife (Minjee Kim) and son (Hanwhi Cho) who are the delayers of my research and the prime movers of my life

Preface

Viscoelasticity or rheology is important in polymer science and engineering because it plays a crucial role in production and characterization of polymeric materials. Understanding the viscoelasticity of polymers requires knowledge of various disciplines such as continuum mechanics, thermodynamics, advanced applied mathematics, polymer physics, and statistical mechanics. Rheology of polymers is studied by the researchers from various fields such as polymer scientists, mechanical engineers, chemical engineers, physicists, and chemists. Hence, it is hard to expect that a newcomer to the field of polymer viscoelasticity would be familiar with such diverse disciplines. From this viewpoint, one may feel the necessity of a book which addresses basic sciences for polymer viscoelasticity as possible as many. Examples of such comprehensive books of rheology are "Dynamics of Polymeric Liquids, volume I and II" written by Bird and coauthors, and "Engineering Rheology" written by Tanner. The book of Bird and coauthors does not contain numerical methods for nonlinear viscoelastic flows while the book of Tanner deals with it. Even though both books are comprehensive rheology books, in the author's opinion, the former is focused on development of constitutive equation while the latter is oriented to the application of constitutive equation to polymer processing. Because it is practically impossible to write a comprehensive book of rheology which contains everything of rheology, most famous books of rheology have their own orientation indicating authors' expertise, with addressing sufficient amount of basic knowledges. The author intends to write a comprehensive rheology book with the orientation to the identification of the rheological properties of polymers from their experimental data. This has been one of the themes of the author's research for recent 10 years.

Any single book cannot satisfy all readers because each reader has different backgrounds and different maturity in their knowledge. When the author was a master-degree student, he thought that Larson's book, "Constitutive Equations of Polymer Melts and Solutions," is not good because it is so compact. However, when he read the book after his Ph.D., he recognized that it is one of well-made rheology books. The present book assumes the readers to have strong background

of engineering mathematics of undergraduate level. The readers do not have to be familiar with tensor analysis because it is given in the book. This book is designed for experimental rheologists, who are strong in mathematics, as well as for students, who want to be familiar with theoretical rheology.

The book consists of three parts. The first part provides fundamental principles which should be necessary to understand the other parts: linear and nonlinear viscoelasticity. This part briefly addresses necessary mathematics, continuum mechanics and thermodynamics, statistical mechanics and polymer physics.

As the book is oriented to the rheological identification of polymers from the experimental data, the second part of linear viscoelasticity contains basic numerical methods which are useful for viscoelastic spectrum, time–temperature superposition, and application of linear viscoelastic principles to polymeric systems. Different from previous rheology books, this part is devoted to numerical algorithms of data processing which is expected to be helpful for experimentalists.

The last part starts from theory of nonlinear constitutive equation in order to explain large amplitude oscillatory shear (LAOS). The last chapter on LAOS is one of the most remarkable features of this book which makes the book different from previous well-made books of rheology.

The author appreciates for the help of a number of persons: his teachers, colleagues, students, and family. Without their help, this book could not have been written. Professor Jinyoung Park, Dongchoon Hyun, Dongyoon Lee, and Dr. Jung-Eun Bae are thankful for the review of the manuscript. Several parts of the book have resulted from the research with my old student, Dr. Jung-Eun Bae. Work cannot be in isolation. The author owes the present work to his teachers who taught him. Especially, Prof. Sangyong Kim made him to recognize the pleasure of academic career. The author cannot forget his students because his research results included in the book cannot be obtained without their assistance. This book was supported by Kyungpook National University Research Fund 2011.

Daegu, Korea Kwang Soo Cho

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Abstract This chapter addresses mathematical preliminaries necessary to understand polymer viscoelasticity assuming that the readers are familiar with engineering mathematics of sophomore. Analysis of vector and tensor is the majority of this chapter, which is necessary to understand constitutive theories of polymer viscoelasticity as well as the theory of polymer physics. Since the knowledge of functional analysis is also needed to understand numerical methods to be used for the processing of viscoelastic data, the vectors and tensors in this chapter include not only physical quantities but also generalized ones called abstract vectors. Because of this purpose, the analysis of vector and tensor starts from the notion of vector space which is an abstraction of physical vector. As for linear viscoelastic theory, both Fourier and Laplace transforms are frequently used. Since this book is not a text of mathematics, rigorous proofs will not be seriously considered. For the proofs, the readers should refer the related references.

1 Vector Space

1.1 Definition of Vector Space

Vector is defined as a quantity having both magnitude and direction as described in undergraduate text books. Although this definition is simple and intuitive, it is not convenient for the application to more general cases. Hence, we will adopt the abstraction of vector which is helpful for the description of the analysis of nonlinear viscoelasticity and the numerical methods of viscoelastic characterization in a unified manner.

One of the most intuitive examples of vector is a displacement vector which points from a position to another position. The sum of two displacement vectors is the vector obtained by parallelogram rule. This rule works for velocity and acceleration obtained by the differentiation of position vector which can be considered as a displacement vector issuing from the origin. Geometric consideration shows easily that velocity and acceleration follows the sum rule of displacement vector.

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However, experiment is needed to prove that force follows the sum rule of displacement vectors, though force has both magnitude and direction. The experimental proof is as simple as to show that when three forces exerted on a point are in equilibrium, the geometric sum of any set of two forces is equal to the opposite of the other force. Here, the opposite of a force is the vector having the same magnitude but opposite direction. Then, one becomes to know that every physical quantity considered as a vector follows the sum rule of displacement vector. As for displacement vector, scalar multiplication is defined as the replacement of the magnitude of the vector by the multiplication of the magnitude by the scalar but maintaining direction. These two binary operations can be used as the generalization of vector.

A set having the two binary operations called addition and scalar multiplication is called a vector space when the two binary operations satisfy the followings and the elements of the set are called vectors.

[1] Addition is commutative:

$$\mathbf{a}+\mathbf{b}=\mathbf{b}+\mathbf{a} \tag{1.1}$$

[2] As for three arbitrary vectors **u**, **v**, **w**, addition is associative:

$$(\mathbf{u}+\mathbf{v})+\mathbf{w}=\mathbf{u}+(\mathbf{v}+\mathbf{w}) \tag{1.2}$$

[3] The zero vector **0** is a unique vector such that for any vector **a**,

$$\mathbf{a}+\mathbf{0}=\mathbf{a} \tag{1.3}$$

[4] For every element of the set, there exists a unique vector $-\mathbf{a}$ such that

$$\mathbf{a}+(-\mathbf{a})=\mathbf{0} \tag{1.4}$$

[5] For any real number c and arbitrary vectors **a** and **b,** the scalar multiplication satisfies

$$c(\mathbf{a}+\mathbf{b})=c\mathbf{a}+c\mathbf{b} \tag{1.5}$$

[6] For any real numbers c and k, scalar multiplication on **a** satisfies

$$(c+k)\mathbf{a}=c\mathbf{a}+k\mathbf{a} \tag{1.6}$$

[7] Associate rule for scalar multiplication is valid for any two scalars c and k and a vector **a**:

$$c(k\mathbf{a})=(ck)\mathbf{a} \tag{1.7}$$

[8] Real number, unity is the identity of the scalar multiplication:

$$1\mathbf{a} = \mathbf{a} \tag{1.8}$$

Note that it is assumed that addition of any two elements of the set is also an element of the set and scalar multiplication of a vector also belongs to the set. More generally, complex number can replace the role of real number. However, we will not treat complex vector space, here, which involves complex number as scalar, because the complex vector is not relevant in mechanics of viscoelasticity.

It is easy to know that the set of continuous functions satisfies the definition of vector space and so does the set of matrices with the same form. Then, continuous function and matrix can be considered as abstract vector.

An example of a vector space, consider pairs of n real numbers denoted by $\mathbf{x} = (x_1, x_2, \ldots, x_n)$. Denote the set of all pairs of n real numbers as E^n. The set is a vector space when addition and scalar multiplication are defined as

$$\begin{aligned} \mathbf{x} + \mathbf{y} &= (x_1 + y_1, x_2 + y_2, \ldots, x_n + y_n) \in E^n \\ c\mathbf{x} &= (cx_1, cx_2, \ldots, cx_n) \in E^n \end{aligned} \tag{1.9}$$

It is easy to prove that E^n satisfies Eqs. (1.1)–(1.8). The vector space E^n is called n-dimensional Euclidean space. An $N \times M$ matrix is considered as a vector of E^{NM}, too.

1.2 Linear Combination and Basis

When m vectors, say, $\mathbf{a}_1, \ldots, \mathbf{a}_m$ are members of a vector space, a vector $\mathbf{x}$ is called a linear combination of the vectors $\mathbf{a}_1, \ldots, \mathbf{a}_m$, if there exist scalars $c_1, c_2, \ldots, c_m$ such that

$$\mathbf{x} = c_1\mathbf{a}_1 + \cdots + c_m\mathbf{a}_m \tag{1.10}$$

When making all of $c_1, c_2, \ldots, c_m$ zero is the only way to make the vector $\mathbf{x}$ of Eq. (1.10) the zero vector, the vectors $\mathbf{a}_1, \ldots, \mathbf{a}_m$ are said to be independent.

Suppose that N vectors $\mathbf{a}_1, \ldots, \mathbf{a}_N$ of a vector space are independent. If any set consisting of the N vectors $\mathbf{a}_1, \ldots, \mathbf{a}_N$ and any other vector of the vector space is not independent, then the N vector $\mathbf{a}_1, \ldots, \mathbf{a}_N$ are called the bases of the vector space. Then, any vector $\mathbf{b}$ and the N vectors $\mathbf{a}_1, \ldots, \mathbf{a}_N$ are not independent. This implies that there exists nonzero real numbers among $c_1, c_2, \ldots, c_{N+1}$ such that

$$c_1\mathbf{a}_1 + \cdots + c_N\mathbf{a}_N + c_{N+1}\mathbf{b} = \mathbf{0} \tag{1.11}$$

If $c_{N+1} = 0$, then Eq. (1.11) means

$$c_1\mathbf{a}_1 + \cdots + c_N\mathbf{a}_N = \mathbf{0} \tag{1.12}$$

and then it is contradictory to the premise that $\mathbf{a}_1, \ldots, \mathbf{a}_N$ are independent. Hence, c_{N+1} must not be zero. Finally, we can express $\mathbf{b}$ as a linear combination of the bases $\mathbf{a}_1, \ldots, \mathbf{a}_N$:

$$\mathbf{b} = -\frac{c_1}{c_{N+1}}\mathbf{a}_1 - \cdots - \frac{c_N}{c_{N+1}}\mathbf{a}_N \tag{1.13}$$

Equation (1.13) implies that any vector of the vector space can be expressed by a linear combination of the base vectors $\mathbf{a}_1, \ldots, \mathbf{a}_N$. That is, an arbitrary vector $\mathbf{v}$ of the vector space can be expressed by

$$\mathbf{v} = \sum_{n=1}^{N} v_n\mathbf{a}_n \tag{1.14}$$

The scalars v_n are called the components of the vector $\mathbf{v}$ with respect to the base vectors of $\{\mathbf{a}_1, \ldots, \mathbf{a}_N\}$. Equation (1.14) implies that basis $\{\mathbf{a}_1, \ldots, \mathbf{a}_N\}$ spans the vector space because any vector can be expressed by a linear combination of the base vectors.

A set of base vectors is called simply basis and a base vector is called a base. There are a number of ways to choose a basis. However, it can be proven that the number of base vectors is not different from each other. The number of base vectors is called the dimension of the vector space. In summary, base vectors have two properties:

[1] Base vectors are linearly independent.
[2] Any vector is expressed by a linear combination of base vectors.

When a set of base vectors of a vector space is known, the two properties of base vectors imply the components of a vector are uniquely determined. Assume that $\{\mathbf{a}_1, \ldots, \mathbf{a}_N\}$ is the set of the base vectors and a vector $\mathbf{v}$ can be expressed by two sets of components as follows:

$$\mathbf{v} = \sum_{n=1}^{N} v_n\mathbf{a}_n = \sum_{n=1}^{N} v'_n\mathbf{a}_n \tag{1.15}$$

Then, Eq. (1.15) leads to

$$\sum_{n=1}^{N} \left(v_n - v'_n\right)\mathbf{a}_n = \mathbf{0} \tag{1.16}$$

Since base vectors are linearly independent, it is clear that for all n, $v_n = v'_n$ which proves that components of a vector are uniquely determined. However, this does not mean that two sets of components of a vector with respect to two different sets of base vectors are identical.

For physical vector in 3-dimensional space, these theoretical tools such as linear independence and base vectors look unnecessarily complicate. However, these concepts are very convenient and necessary when abstract vectors such as continuous functions are considered. The approaches based on vector space can be met in several fields of applied mathematics as well as quantum mechanics. See Atkinson and Han (2000) for numerical methods, and Luenberger (1969) for optimization theory, Kreyszig (1978) for functional analysis, and Prugovecki (2006) for quantum mechanics.

A vector space can have a number of base vectors. A new set of N vectors can be generated by linear combination of a set of base vectors $A = \{\mathbf{a}_1, \ldots, \mathbf{a}_N\}$ as follows:

$$\mathbf{b}_i = \sum_{k=1}^{N} Q_{ik}\mathbf{a}_k \quad (i = 1, 2, \ldots, N) \tag{1.17}$$

where coefficients Q_{ik} are assumed to form an invertible matrix. Consider a linear combination from $B = \{\mathbf{b}_1, \ldots, \mathbf{b}_N\}$: $\mathbf{u} \equiv c_1\mathbf{b}_1 + \cdots + c_N\mathbf{b}_N$. If the vector $\mathbf{u}$ is the zero vector, then we have

$$\mathbf{u} = \sum_{i=1}^{N} c_i\mathbf{b}_i = \sum_{i=1}^{N} c_i \left(\sum_{k=1}^{N} Q_{ik}\mathbf{a}_k \right) = \sum_{k=1}^{N} \left(\sum_{i=1}^{N} Q_{ik}c_i \right) \mathbf{a}_k = \mathbf{0} \tag{1.18}$$

Equation (1.18) implies that for all k

$$\sum_{i=1}^{N} Q_{ik}c_i = 0 \tag{1.19}$$

Since the matrix Q_{ik} is invertible, Eq. (1.19) uniquely determines $c_i = 0$ for all i. Hence, the set $\{\mathbf{b}_i\}$ is linearly independent. Let P_{mn} be the inverse matrix of Q_{ik}. Then, we have

$$\mathbf{a}_i = \sum_{k=1}^{N} P_{ik}\mathbf{b}_k \quad (i = 1, 2, \ldots, N) \tag{1.20}$$

Substitution of Eq. (1.20) into Eq. (1.14) proves that any vector $\mathbf{v}$ can be expressed by a linear combination of $B = \{\mathbf{b}_1, \ldots, \mathbf{b}_N\}$. Detailed proofs are found in Ames (1970).

1.3 Dual Space

Consider a linear mapping $\widetilde{\phi}$ from a vector space V to real numbers. It is a real-valued function of a vector of V with satisfying the following properties:

$$\widetilde{\phi}(\mathbf{u}+\mathbf{v}) = \widetilde{\phi}(\mathbf{u}) + \widetilde{\phi}(\mathbf{v}), \quad \widetilde{\phi}(\alpha\mathbf{u}) = \alpha\widetilde{\phi}(\mathbf{u}) \tag{1.21}$$

where α is an arbitrary real number and $\mathbf{u}$ and $\mathbf{v}$ are arbitrary vectors of V. The linear mapping $\widetilde{\phi}$ is called linear functional. If a set of linear functionals on V satisfies the conditions of vector space, then the set is denoted by V^* and called the dual space of the vector space V.

Here, the addition of any two functionals $\widetilde{\phi} \in V^*$ and $\widetilde{\eta} \in V^*$ is defined as

$$\left(\widetilde{\phi} + \widetilde{\eta}\right)(\mathbf{u}) \equiv \widetilde{\phi}(\mathbf{u}) + \widetilde{\eta}(\mathbf{u}) \tag{1.22}$$

Then, it is clear that $\widetilde{\phi} + \widetilde{\eta} \in V^*$. For any real number α, scalar multiplication is defined as

$$\left(\alpha\widetilde{\phi}\right)(\mathbf{u}) \equiv \alpha\widetilde{\phi}(\mathbf{u}) \tag{1.23}$$

Of course, we know that $\alpha\widetilde{\phi} \in V^*$. The zero functional is defined a mapping from V to 0 for any elements of V. Then, it is not difficult to show that the set of linear functional V^* is a vector space.

Let $\{\mathbf{b}_i\}$ be a set of base vectors of N-dimensional vector space V. Consider N linear functionals $\widetilde{\phi}^{(i)}$ defined as $\widetilde{\phi}^{(i)}(\mathbf{b}_k) = \delta_{ik}$ where δ_{ik} is the *Kronecker's delta* which is unity whenever $i = k$ and zero otherwise. Then, it is easy to show that the set $\{\widetilde{\phi}^{(i)}\}$ is the base of V^*. The first step is to show that $\{\widetilde{\phi}^{(i)}\}$ is linearly independent and the second step is to show that $\{\widetilde{\phi}^{(i)}\}$ generates any linear functional that belongs to V^*. The linear independence of $\{\widetilde{\phi}^{(i)}\}$ means that if a linear combination of $\{\widetilde{\phi}^{(i)}\}$ for any vector $\mathbf{v}$ of V is zero:

$$\sum_{k=1}^{N} c_k \widetilde{\phi}^{(k)}(\mathbf{v}) = 0 \tag{1.24}$$

then all coefficients c_k are zero. Substitution of a base vector $\mathbf{b}_i$ of V to Eq. (1.24) gives $c_i = 0$. Thus, the set $\{\widetilde{\phi}^{(i)}\}$ is linearly independent. For any vector $\mathbf{v}$ whose components are v_k, a linear functional $\widetilde{\phi}$ satisfies

$$\widetilde{\phi}(\mathbf{v}) = \widetilde{\phi}\left(\sum_{k=1}^{N} v_k \mathbf{b}_k\right) = \sum_{k=1}^{N} v_k \widetilde{\phi}(\mathbf{b}_k) \tag{1.25}$$

Equation (1.25) implies that if N values of $\widetilde{\phi}(\mathbf{b}_i)$ are known, then the value of $\widetilde{\phi}(\mathbf{v})$ is determined. Consider a functional $\widetilde{\psi}$ which is a linear functional such that

$$\widetilde{\psi}(\mathbf{v}) = \sum_{k=1}^{N} \widetilde{\phi}(\mathbf{b}_k)\widetilde{\phi}^{(k)}(\mathbf{v}) \tag{1.26}$$

Then, we know that $\psi(\mathbf{b}_i) = \widetilde{\phi}(\mathbf{b}_i)$ from the definition of $\widetilde{\phi}^{(i)}$. It is clear that the functional $\widetilde{\psi}(\mathbf{v})$ is identical to $\widetilde{\phi}(\mathbf{v})$ because the two linear functionals have the same value for any vector $\mathbf{v}$.

The Dirac delta function is one of the most important applications of linear functional. Consider the vector space F of continuous functions defined on the interval $(-\infty, \infty)$. One may define linear functional by using the following integral transform

$$\widetilde{\phi}[f(x)] = \int_{-\infty}^{\infty} \phi(x) f(x) \mathrm{d}x \tag{1.27}$$

where $f(x)$ is a vector of F and $\phi(x)$ is the function given by the functional $\widetilde{\phi}$. The function $\phi(x)$ can be considered as the kernel function from the viewpoint of integral transform. Fourier transform is a linear functional for functions $f(x)$ which satisfies

$$\int_{-\infty}^{\infty} |f(x)| \mathrm{d}x < \infty \tag{1.28}$$

and the kernel function is given by $\phi(x) = \exp(-\mathrm{i}qx)$ where $\mathrm{i} = \sqrt{-1}$. One may imagine that any linear functional corresponds to its own kernel function: the one-to-one correspondence between linear functional and function. The existence of the correspondence can be proved when the inner product is defined over the vector space of functions. It will be treated later. The Dirac delta function is the kernel function of the linear functional which maps $f(x) \in F$ to $f(0)$:

$$\widetilde{\delta}[f(x)] = \int_{-\infty}^{\infty} \delta(x) f(x) \mathrm{d}x = f(0) \tag{1.29}$$

However, the Dirac delta function $\delta(x)$ cannot be defined at $x = 0$. Hence, new name for something like function is necessary. The name is distribution (Zemanian 1987). Note that $\delta(x)$ works always under integration. Thus, the Dirac delta function can be said to be a linear functional.

Problem 1

[1] Show that the following sets are vector space if addition and scalar multiplication are suitably defined.

[a] Set of $N \times M$ matrix,
[b] Set of polynomials of order N,
[c] Set of linear functionals from physical vectors.

[2] Show that the followings are linearly independent.

[a] $\{\sin \omega t, \sin 2\omega t, \sin 3\omega t, \ldots, \sin N\omega t\}$
[b] $\left\{1, x, x^2, x^3, \ldots, x^N\right\}$

[3] When $B = \{\mathbf{b}_1, \mathbf{b}_2, \ldots, \mathbf{b}_N\} \subset V$ is a linearly independent set of vector space V, show that any subset of B is also linearly independent.

[4] If $\{\mathbf{a}_1, \mathbf{a}_2, \ldots, \mathbf{a}_N\}$ is a base of vector space V and $\{\mathbf{b}_1, \mathbf{b}_2, \ldots, \mathbf{b}_M\}$ is also a base of the same vector space, then show that $M = N$.

[5] If a subset of a vector space V is also a vector space, then it is called subspace. Consider two subspace V_1 and V_2 of V. Show that the following set is a vector space.

$$V_1 + V_2 \equiv \{\mathbf{v} | \mathbf{v} = \mathbf{v}_1 + \mathbf{v}_2; \mathbf{v}_1 \in V_1, \mathbf{v}_2 \in V_2\}$$

[6] Show that the intersection of two subspace is a vector space.

[7] V_1 and V_2 are subspaces of V whose dimension is finite. When the dimension of a vector space U is denoted by $\dim(U)$, show that

$$\dim(V_1 + V_2) = \dim(V_1) + \dim(V_2) - \dim(V_1 \cap V_2)$$

2 Inner Product Space

2.1 Generalization of Inner Product

In physics, the inner product of two vectors is defined as the product of three terms: the magnitudes of the two vectors and the cosine of the angle between the two vectors. Hence, the inner product can be considered as a mapping from two vectors to a real number. It is assumed that the readers are familiar with the inner product of physics. Then, it is clear that

$$\begin{aligned} \mathbf{a}\cdot\mathbf{b} &= \mathbf{b}\cdot\mathbf{a} \\ (\mathbf{a}+\mathbf{b})\cdot\mathbf{c} &= \mathbf{a}\cdot\mathbf{c}+\mathbf{b}\cdot\mathbf{c} \\ (k\mathbf{a})\cdot\mathbf{b} &= k(\mathbf{a}\cdot\mathbf{b}) \\ \mathbf{a}\cdot\mathbf{a} &\geq 0 \end{aligned} \tag{2.1}$$

where **a**, **b**, and **c** are arbitrary vectors and k is an arbitrary real number. Note that $\mathbf{a}\cdot\mathbf{a}=0$ is valid only when $\mathbf{a}=\mathbf{0}$. Furthermore, we know that the magnitude of a vector **a** is given by

$$\|\mathbf{a}\| = \sqrt{\mathbf{a}\cdot\mathbf{a}} \tag{2.2}$$

Generalization of inner product can be done by the replacement of the physical vectors in Eq. (2.1) by abstract ones of arbitrary vector space. In other words, we define inner product as a binary operation satisfying Eq. (2.1). The notation $\langle \mathbf{a}, \mathbf{b}\rangle$ instead of $\mathbf{a}\cdot\mathbf{b}$ would be used in order to emphasize that the inner product under consideration is a generalized one. There are a number of definitions of inner product available for a given vector space.

Consider a vector space consisting of integrable functions on the interval of $[a, b]$. Then, one of the simplest inner product might be defined as

$$\langle f, g\rangle \equiv \int_a^b f(x)g(x)w(x)\mathrm{d}x \tag{2.3}$$

where $w(x)$ is nonnegative over the interval and called weight function. It is easy to show that Eq. (2.3) satisfies Eq. (2.1).

As for $N \times N$ matrix, one may define inner product as follows:

$$\langle \mathbf{A}, \mathbf{B}\rangle \equiv \sum_{i=1}^{N}\sum_{k=1}^{N} a_{ik}b_{ik} \tag{2.4}$$

where **A** and **B** are $N \times N$ matrices and a_{ik} and b_{ik} are their components, respectively. It is also easy to show that Eq. (2.4) satisfies Eq. (2.1).

A vector space with inner product is called inner product space and the magnitude of vector is called *norm*. Metric space is a vector space equipped with the definition of norm. Since the norm of vector can be defined from inner product, inner product space is a metric space. If every *Cauchy sequence* of vectors of an inner product space converges in the space, then the space is called *Hilbert space* irrespective of the dimension of the space. A sequence of vectors $\{\mathbf{x}_k\}$ is a Cauchy sequence when it satisfies the condition that if for any positive real number $\varepsilon > 0$, there exists a positive integer N such that for all positive integers $m, n > N$, then the magnitude of $\mathbf{x}_m - \mathbf{x}_n$ is smaller than ε. Since we can take linear combinations of base vectors as a sequence, and any vector of the Hilbert space can be expressed by

a linear combination of base vectors, it is clear that any inner product space of finite dimension is a Hilbert space. However, all inner product spaces of infinite dimension are not Hilbert spaces. Further information on metric and Hilbert spaces are found in Kreyszig (1978), Luenberger (1969), and Prugovecki (2006).

2.2 Generalization of Distance

The distance between two positions is equal to the magnitude of the displacement vector connecting the two positions. The magnitude of a geometric vector can be obtained by the inner product as shown in Eq. (2.2). Then, the distance in a metric space can be defined as the norm of the difference between two vectors of the metric space.

The notion of distance in our daily life is summarized with *the nonnegativity of distance* that the distance between any two vectors is nonnegative; *the symmetry of distance* that the distance from **a** to **b** is equal to that from **b** to **a**; *the triangle inequality* that the sum of distances from **a** to **b** and from **b** to **c** is not less than the distance between **a** and **c**. If the distance between **a** and **b** is denoted by $g(\mathbf{a}, \mathbf{b})$, then the three axioms are expressed by

$$\begin{aligned} &g(\mathbf{a}, \mathbf{b}) \geq 0 \\ &g(\mathbf{a}, \mathbf{b}) = g(\mathbf{b}, \mathbf{a}) \\ &g(\mathbf{a}, \mathbf{b}) + g(\mathbf{b}, \mathbf{c}) \geq g(\mathbf{a}, \mathbf{c}) \end{aligned} \tag{2.5}$$

As for inner product space, one can define the distance from inner product as $g(\mathbf{a}, \mathbf{b}) \equiv \sqrt{\langle \mathbf{a} - \mathbf{b}, \mathbf{a} - \mathbf{b} \rangle}$. Then, it is not difficult to show that the definition of distance satisfies Eq. (2.5) except the triangle inequality. The Cauchy–Schwarz inequality is necessary to prove the triangle inequality. For any generalized inner product which satisfies Eq. (2.1), the following is valid:

$$\langle \mathbf{a}, \mathbf{a} \rangle \langle \mathbf{b}, \mathbf{b} \rangle \geq \langle \mathbf{a}, \mathbf{b} \rangle^2 \tag{2.6}$$

where **a** and **b** are arbitrary vectors of an inner product space. Because of the last inequality of Eq. (2.1), for any real number t, we have

$$\langle \mathbf{a} + t\mathbf{b}, \mathbf{a} + t\mathbf{b} \rangle \geq 0 \tag{2.7}$$

Applying the properties of inner product, Eq. (2.7) can be rewritten as

$$\langle \mathbf{b}, \mathbf{b} \rangle t^2 + 2\langle \mathbf{a}, \mathbf{b} \rangle t + \langle \mathbf{a}, \mathbf{a} \rangle \geq 0 \tag{2.8}$$

Since Eq. (2.8) is valid for any real number, the discriminant must not be positive:

$$\frac{D}{4} = \langle \mathbf{a}, \mathbf{b} \rangle^2 - \langle \mathbf{a}, \mathbf{a} \rangle \langle \mathbf{b}, \mathbf{b} \rangle \leq 0 \tag{2.9}$$

Note that Eq. (2.9) is identical to Eq. (2.6).

As for physical vector, the Cauchy–Schwarz inequality is straightforward because of the definition of the inner product in physics such that

$$\langle \mathbf{a}, \mathbf{b} \rangle = \mathbf{a} \cdot \mathbf{b} = \|\mathbf{a}\| \|\mathbf{b}\| \cos\theta \tag{2.10}$$

where θ is the angle between the two vectors. Note that $-1 \leq \cos\theta \leq 1$ for any θ. Analogy to the inner product of physical vectors, the angle between two abstract vectors might be defined as

$$\cos\theta \equiv \frac{\langle \mathbf{a}, \mathbf{b} \rangle}{\sqrt{\langle \mathbf{a}, \mathbf{a} \rangle} \sqrt{\langle \mathbf{b}, \mathbf{b} \rangle}} \tag{2.11}$$

Let us move back to the problem of the triangle inequality of distance. Since distance is not negative, the triangle inequality is equivalent to

$$[g(\mathbf{a}, \mathbf{b}) + g(\mathbf{b}, \mathbf{c})]^2 \geq [g(\mathbf{a}, \mathbf{c})]^2 \tag{2.12}$$

Replace the distance function by the corresponding inner product. Then, we have

$$\begin{aligned} [g(\mathbf{a},\ \mathbf{b}) + g(\mathbf{b}, \mathbf{c})]^2 &\geq \langle \mathbf{a} - \mathbf{b}, \mathbf{a} - \mathbf{b} \rangle + \langle \mathbf{b} - \mathbf{c}, \mathbf{b} - \mathbf{c} \rangle + 2\langle \mathbf{a} - \mathbf{b}, \mathbf{b} - \mathbf{c} \rangle \\ &= \langle (\mathbf{a} - \mathbf{b}) + (\mathbf{b} - \mathbf{c}), (\mathbf{a} - \mathbf{b}) + (\mathbf{b} - \mathbf{c}) \rangle = \langle \mathbf{a} - \mathbf{c}, \mathbf{a} - \mathbf{c} \rangle \\ &= [g(\mathbf{a}, \mathbf{c})]^2 \end{aligned} \tag{2.13}$$

Then, the proof is completed.

2.3 *Orthogonalized Basis*

Vector spaces considered in this book are usually assumed as inner product space or Hilbert space. From inner product, one can consider the notion of orthogonality such that the inner product of two nonzero vector is zero. As for physical vectors, orthogonality implies that the directions of the two vectors are perpendicular to each other. Hence, orthogonality is an abstraction of the perpendicularity of geometry. Whenever we consider physical vectors, orthogonality is identical to perpendicularity.

In general, two base vectors do not have to be orthogonal. However, mutually orthogonal base vectors are more convenient. Consider N mutually orthogonal

vectors of an inner product space of finite dimension. These vectors are linearly independent if N is not larger than the dimension of the inner product space. Mutually orthogonal vectors $\{\mathbf{u}_1, \mathbf{u}_2, \ldots, \mathbf{u}_N\}$ are said to be vectors such that $\langle \mathbf{u}_i, \mathbf{u}_k \rangle = 0$ for any pair of i and k whenever the two indices are not same. If a linear combination of these vectors is the zero vector:

$$c_1\mathbf{u}_1 + c_2\mathbf{u}_2 + \cdots + c_N\mathbf{u}_N = \mathbf{0} \tag{2.14}$$

then taking inner product with $\mathbf{u}_i$ on both sides of Eq. (2.14) gives $c_i\langle \mathbf{u}_i, \mathbf{u}_i \rangle = 0$. The property of inner product results in $c_i = 0$ for any i. Thus, these N vectors are linearly independent. It is not difficult to show that contradiction occurs whenever N is larger than the dimension of the space. If N is equal to the dimension of the space, it is clear that the N mutually orthogonal vectors are base vectors.

Mutually orthogonal base vectors are called orthonormal base vectors when every member of the base vectors has the magnitude of unity. If we have mutually orthogonal base vectors $\{\mathbf{u}_1, \mathbf{u}_2, \ldots, \mathbf{u}_N\}$, then we can define N vectors such that

$$\mathbf{e}_i = \frac{1}{\sqrt{\langle \mathbf{u}_i, \mathbf{u}_i \rangle}}\mathbf{u}_i \quad \text{for} \quad i = 1, 2, \ldots, N \tag{2.15}$$

From Eq. (2.15), it is straightforward that

$$\langle \mathbf{e}_i, \mathbf{e}_k \rangle = \mathbf{e}_i \cdot \mathbf{e}_k = \delta_{ik} \tag{2.16}$$

where δ_{ik} is called Kronecker's delta which is unity when $i = k$ and zero otherwise. Orthonormal base vectors are more convenient than mutually orthogonal ones because any vector can be expressed by

$$\mathbf{v} = \sum_{k=1}^{N} \langle \mathbf{v}, \mathbf{e}_k \rangle \mathbf{e}_k = \sum_{k=1}^{N} (\mathbf{v} \cdot \mathbf{e}_k)\mathbf{e}_k \tag{2.17}$$

When orthonormal base is used, inner product of any two vectors is expressed by

$$\langle \mathbf{a}, \mathbf{b} \rangle = \mathbf{a} \cdot \mathbf{b} = \sum_{k=1}^{N} a_k b_k \tag{2.18}$$

where a_k and b_k are kth components of $\mathbf{a}$ and $\mathbf{b}$, respectively, with respect to the orthonormal base.

Then, how can we obtain an orthonormal base from a given base? Suppose that we have a basis $\{\mathbf{b}_1, \mathbf{b}_2, \ldots, \mathbf{b}_N\}$, which do not have to be mutually orthogonal. Since a member of an orthogonal basis $\{\mathbf{e}_1, \mathbf{e}_2, \ldots, \mathbf{e}_N\}$ is also a vector, it can be expressed by a linear combination of $\{\mathbf{b}_1, \mathbf{b}_2, \ldots, \mathbf{b}_N\}$:

$$\mathbf{e}_i = \sum_{k=1}^{N} Q_{ik}\mathbf{b}_k \tag{2.19}$$

With the help of Eq. (2.16), we have

$$\left\langle \sum_{n=1}^{N} Q_{in}\mathbf{b}_n, \sum_{m=1}^{N} Q_{km}\mathbf{b}_m \right\rangle = \sum_{n=1}^{N}\sum_{m=1}^{N} Q_{in}Q_{km}\langle \mathbf{b}_n, \mathbf{b}_m\rangle = \delta_{ik} \tag{2.20}$$

Since we know $\langle \mathbf{b}_n, \mathbf{b}_m\rangle$ for any pair of n and m, Eq. (2.20) is a set of N^2 nonlinear equations for N^2 unknowns Q_{ik}. This is a quite complicate problem. The *Gram–Schmidt orthogonalization* is a simpler method to find Q_{ik} in a systematic way.

2.3.1 The Gram–Schmidt Orthogonalization

The first step of the Gram–Schmidt orthogonalization is to find a mutually orthogonal bias, say $\{\mathbf{u}_1, \mathbf{u}_2, \ldots, \mathbf{u}_N\}$ from a given basis $\{\mathbf{b}_1, \mathbf{b}_2, \ldots, \mathbf{b}_N\}$. The next step is the normalization of the mutually orthogonal basis by $\mathbf{e}_i = \mathbf{u}_i/\|\mathbf{u}_i\|$.

Set $\mathbf{u}_1 = \mathbf{b}_1$ and $\mathbf{u}_2 = \mathbf{b}_2 + q_1^{(2)}\mathbf{u}_1$. Then, there is only one unknown $q_1^{(2)}$ which could be determined by the orthogonality condition of $\langle \mathbf{u}_1, \mathbf{u}_2\rangle = 0$. Then, we know that

$$q_1^{(2)} = -\frac{\langle \mathbf{b}_2, \mathbf{b}_1\rangle}{\langle \mathbf{b}_1, \mathbf{b}_1\rangle} = -\frac{\langle \mathbf{b}_2, \mathbf{u}_1\rangle}{\langle \mathbf{u}_1, \mathbf{u}_1\rangle} \tag{2.21}$$

Since there are two orthogonal conditions such that $\langle \mathbf{u}_1, \mathbf{u}_3\rangle = 0$ and $\langle \mathbf{u}_2, \mathbf{u}_3\rangle = 0$, one may construct $\mathbf{u}_3$ by $\mathbf{u}_3 = \mathbf{b}_3 + q_2^{(3)}\mathbf{u}_2 + q_1^{(3)}\mathbf{u}_1$. The unknowns $q_2^{(3)}$ and $q_1^{(3)}$ can be determined by solving the following set of linear equations:

$$\begin{aligned} \langle \mathbf{u}_1, \mathbf{u}_1\rangle q_1^{(3)} + \langle \mathbf{u}_1, \mathbf{u}_2\rangle q_2^{(3)} &= -\langle \mathbf{u}_1, \mathbf{u}_3\rangle \\ \langle \mathbf{u}_2, \mathbf{u}_1\rangle q_1^{(3)} + \langle \mathbf{u}_2, \mathbf{u}_2\rangle q_2^{(3)} &= -\langle \mathbf{u}_2, \mathbf{u}_3\rangle \end{aligned} \tag{2.22}$$

Since $\langle \mathbf{u}_k, \mathbf{u}_k\rangle > 0$ because $\mathbf{u}_k \neq \mathbf{0}$ for any k, Eq. (2.22) must have a unique solution and we have

$$\mathbf{u}_3 = \mathbf{b}_3 - \frac{\langle \mathbf{b}_3, \mathbf{u}_2\rangle}{\langle \mathbf{u}_2, \mathbf{u}_2\rangle}\mathbf{u}_2 - \frac{\langle \mathbf{b}_3, \mathbf{u}_1\rangle}{\langle \mathbf{u}_1, \mathbf{u}_1\rangle}\mathbf{u}_1 \tag{2.23}$$

Similar procedure can be applied to $\mathbf{u}_n$ for $n > 3$ and we have

$$\mathbf{u}_n = \mathbf{b}_n - \sum_{k=1}^{n-1} \frac{\langle \mathbf{b}_n, \mathbf{u}_k\rangle}{\langle \mathbf{u}_k, \mathbf{u}_k\rangle}\mathbf{u}_k \tag{2.24}$$

Since this procedure gives mutually orthogonal basis $\{\mathbf{u}_1, \mathbf{u}_2, \ldots, \mathbf{u}_N\}$, finally we have orthonormal basis:

$$\mathbf{e}_i = \frac{1}{\|\mathbf{u}_i\|}\mathbf{u}_i \tag{2.25}$$

The Gram–Schmidt orthogonalization implies that any inner product space can have orthonormal basis. We know that finite-order polynomials have the basis $B_N = \{1, x, \ldots, x^N\}$. Suppose that the inner product space of polynomial is equipped with the inner product defined by

$$\langle p(x), q(x)\rangle = \int_a^b p(x)q(x)w(x)\mathrm{d}x \tag{2.26}$$

where the weight function $w(x)$ is positive for the whole interval of $a < x < b$.

First, consider the case of $a = 0$, $b = L > 0$, and $w(x) = 1$, then the mutually orthogonal basis $M_N = \{Q_0(x), Q_1(x), \ldots, Q_N(x)\}$ from the basis B_N is given by

$$Q_0(x) = 1; \quad Q_1(x) = x - \frac{1}{2}L; \quad Q_2(x) = x^2 - Lx + \frac{1}{6}L^2; \quad \ldots \tag{2.27}$$

Note that $M_N \subset M_{N+m}$ when $m > 0$.

2.3.2 Orthogonal Polynomials

There are several named orthogonal polynomials which have different definitions of inner product. The Legendre polynomials construct an orthogonal basis for $a = -1$, $b = 1$ and $w(x) = 1$. Some of the Legendre polynomials are

$$\begin{aligned} &P_0(x) = 1; \quad P_1(x) = x; \quad P_2(x) = 2^{-1}\left(3x^2 - 1\right); \\ &P_3(x) = 2^{-1}\left(5x^3 - 3x\right); \quad P_4(x) = 2^{-3}\left(35x^4 - 30x^2 + 3\right); \\ &P_5(x) = 2^{-3}\left(63x^5 - 70x^3 + 15x\right); \quad \ldots \end{aligned} \tag{2.28}$$

Although the Gram–Schmidt orthogonalization is easy to be understood and is a systematic way, the calculation procedures are tedious and time-consuming. As for the Legendre polynomials, the following recursive equation is valid:

$$P_{n+1}(x) = \frac{2n+1}{n+1}xP_n(x) - \frac{n}{n+1}P_{n-1}(x) \quad \text{for} \quad n \geq 1 \tag{2.29}$$

Note that $P_0(x) = 1$ and $P_1(x) = x$ are needed as initial conditions for the recursive Eq. (2.29). The recursive equations are more convenient than the Gram–

Schmidt orthogonalization. As for the Legendre polynomials, the following orthogonal conditions are valid:

$$\int_{-1}^{1} P_m(x)\, P_n(x)\mathrm{d}x = \frac{2}{2n+1}\delta_{mn} \tag{2.30}$$

When $a = -1$, $b = 1$ and $w(x) = 1/\sqrt{1-x^2}$ is used, the Chebyshev polynomials of the first kind are obtained. Some of the Chebyshev polynomials of the first kind are

$$\begin{aligned} &T_0(x) = 1; \quad T_1(x) = x; \quad T_2(x) = 2x^2 - 1; \\ &T_3(x) = 4x^3 - 3x; \quad T_4(x) = 8x^4 - 8x^2 + 1; \\ &T_5(x) = 16x^5 - 20x^3 + 5x; \ldots \end{aligned} \tag{2.31}$$

The recursive equation for the Chebyshev polynomial of the first kind is given as

$$T_{n+1}(x) = 2xT_n(x) - T_{n-1}(x) \quad \text{for } n \geq 1 \tag{2.32}$$

with the initial conditions of $T_0(x) = 1$ and $T_1(x) = x$. The orthogonal conditions are given as

$$\int_{-1}^{1} \frac{T_m(x)\, T_n(x)}{\sqrt{1-x^2}}\mathrm{d}x = \begin{cases} 0 & \text{for } m \neq n \\ \pi & \text{for } m = n = 0 \\ \frac{1}{2}\pi & \text{for } m = n \neq 0 \end{cases} \tag{2.33}$$

It is noteworthy that the Chebyshev polynomial of the first kind is useful in analysis of large amplitude oscillatory shear (LAOS) because it has the following properties:

$$\begin{aligned} &T_n(\cos\theta) = \cos(n\theta) \\ &T_n(x) = T_n(n \arccos x) = \cosh(n \arccos \mathrm{h}x) \end{aligned} \tag{2.34}$$

See Chap. 11. Furthermore, the Chebyshev polynomial of the first kind is also useful in various fields of numerical methods. Polynomial regression is one of the most representative applications of the polynomial.

The Chebyshev polynomial of the second kind $U_n(x)$ is defined over the same interval, but its weight function is $w(x) = \sqrt{1-x^2}$. Its recursive equation is the same as that of the first kind while the initial conditions are given as $U_0(x) = 1$ and $U_1(x) = 2x$.

The Hermite polynomials are an orthogonal basis for $a = -\infty$, $b = \infty$ and $w(x) = \exp(-x^2)$. Some of the Hermite polynomials are