補遺
Supplement

線形代数セミナー
Seminar on Linear Algebra

—射影，特異値分解，一般逆行列—
Projection, Singular Value Decomposition, Pseudoinverse

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Contents

Chapter 1

Linear Space and Projection

1.1 Expression of Linear Mapping

A linear mapping from the n-dimensional space $\mathcal{R}^n$ to the m-dimensional is represented by an $m \times n$ matrix $\boldsymbol{A}$ ($\hookrightarrow$ Appendix A.1). One of the basic ways to specify it is to define an *orthonormal basis* $\{\boldsymbol{u}_1, ..., \boldsymbol{u}_n\}$, i.e., mutually orthogonal unit vectors, in $\mathcal{R}^n$, which is called the *domain*, and to specify the *image*, $\boldsymbol{a}_1, ..., \boldsymbol{a}_n$, i.e., the m-dimensional vectors to which the basis vectors are to be mapped (Fig. 1.1). Then, the matrix $\boldsymbol{A}$ is written in the form of Eq. (1.1) ($\hookrightarrow$ Problem 1.1), where the symbol $\top$ denotes transpose[1]. In fact, if we multiply Eq. (1.1) by $\boldsymbol{u}_i$ from right, we obtain $\boldsymbol{A}\boldsymbol{u}_i = \boldsymbol{a}_i$ from the orthonormality of Eq. (1.2), where δ_{ij} is the *Kronecker delta*, which takes the value 1 for $j = i$ and 0 for $j \neq i$.

If we use the *natural basis* $\{\boldsymbol{e}_1, ... \boldsymbol{e}_n\}$, where $\boldsymbol{e}_i$ is the n-dimensional vector whose ith component is 1 and whose other components are all 0, the vetor $\boldsymbol{a}_i = (a_{1i}, ..., a_{mi})^\top$ is expressed in the form of Eq. (1.3). In other words, *the matrix $\boldsymbol{A}$ consists of the images $\boldsymbol{a}_1$, ..., $\boldsymbol{a}_n$ as its columns in that order* (Fig. 1.2).

Example. Rotation in two dimensions

Rotation by angle θ (anti-clockwise) in two dimensions is a linear mapping. The natural basis vectors $\boldsymbol{e}_1 = (1, 0)^\top$ and $\boldsymbol{e}_2 = (0, 1)^\top$ are mapped to $\boldsymbol{a}_1 = (\cos\theta, \sin\theta)^\top$ and $\boldsymbol{a}_2 = (-\sin\theta, \cos\theta)^\top$, respectively, after a rotation by angle θ (Fig. 1.3). Hence, rotation by angle θ is represented by the matrix $\boldsymbol{R}(\theta) = \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix}$.

[1] Mathematicians often use the letter "t", the initial of "transpose", as the left superscript to write ${}^{\mathrm{t}}\boldsymbol{u}$ for the transpose of vector $\boldsymbol{u}$, while physicists and engineers usually use the symbol $\top$ as the right superscript to write it as $\boldsymbol{u}^\top$.

1.2 Subspaces, Projection, and Rejection

Let $\boldsymbol{u}_1$, ..., $\boldsymbol{u}_r$ be a set of r linearly independent vectors in the n-dimensional space $\mathcal{R}^n$. The set $\mathcal{U} \subset \mathcal{R}^n$ of all linear combinations of these vectors is called the r-dimensional *subspace spanned by* $\boldsymbol{u}_1$, ..., $\boldsymbol{u}_r$. For instance, the subspace spanned by one vector is a line that extends along it, and the subspace spanned by two vectors is the plane that passes through them.

Given a point P in $\mathcal{R}^n$ and a subpace $\mathcal{U} \subset \mathcal{R}^n$, the point $Q \in \mathcal{U}$ defined so that $\overrightarrow{PQ}$ is orthogonal to $\mathcal{U}$ is called the *projection*[2] of P onto $\mathcal{U}$, and $\overrightarrow{QP}$ is said to be the *rejection* of Q from $\mathcal{U}$ (Fig. 1.4). If we move the point Q to another point Q' of $\mathcal{U}$, we obtain from the Pythagorean theorem ($\hookrightarrow$ Appendix Eq. (A.12)), we obtain Eq. (1.4). In other words, the projection Q is the closest point of $\mathcal{U}$ from point P ($\hookrightarrow$ Problem 1.2).

These facts are summarized in the form of Eq. (1.5), where $\mathcal{U}^\perp$ is the set of all vectors orthogonal to $\mathcal{U}$, called the *orthogonal complement* of $\mathcal{U}$, which is also a subspace of $\mathcal{R}^n$. Thus any vector of $\mathcal{R}^n$ is expressed as the sum of its projection onto $\mathcal{U}$ and the rejection from it. Such an expression is unique and called the *direct sum decomposition* of $\overrightarrow{OP}$ to $\mathcal{U}$ and $\mathcal{U}^\perp$.

1.3 Projection Matrices

Let $\boldsymbol{P}_{\mathcal{U}^\perp}$ be the projection onto subspace $\mathcal{U}$, and $\boldsymbol{P}_{\mathcal{U}^\perp}$ the projection onto its orthogonal complement $\mathcal{U}^\perp$. By definition, Eqs. (1.6) and (1.7) hold. If we define an orthonormal basis $\{\boldsymbol{u}_1, ..., \boldsymbol{u}_r\}$ of the subspace $\mathcal{U}$, it can be extended to an orthonormal basis $\{\boldsymbol{u}_1, ..., \boldsymbol{u}_r, \boldsymbol{u}_{r+1}, ..., \boldsymbol{u}_n\}$ of $\mathcal{R}^n$. Equation (1.6) means that $\boldsymbol{P}_{\mathcal{U}}$ maps the orthonormal basis vectors $\{\boldsymbol{u}_1, ..., \boldsymbol{u}_n\}$ of $\mathcal{R}^n$ to $\boldsymbol{u}_1$, ..., $\boldsymbol{u}_r$, $\boldsymbol{0}$, ..., $\boldsymbol{0}$, respectively. Similarly, Eq. (1.7) means that $\boldsymbol{P}_{\mathcal{U}^\perp}$ maps $\{\boldsymbol{u}_1, ..., \boldsymbol{u}_n\}$ to $\boldsymbol{0}$, ..., $\boldsymbol{0}$, $\boldsymbol{u}_{r+1}$, ..., $\boldsymbol{u}_n$, respectively. Hence, from Eq. (1.1), the mappings $\boldsymbol{P}_{\mathcal{U}}$ and are expressed as matrices in the form of Eqs. (1.8) and (1.9), respectively, where $\boldsymbol{P}_{\mathcal{U}}$ and $\boldsymbol{P}_{\mathcal{U}^\perp}$ are called the *projection matrices* onto subspaces $\mathcal{U}$ and $\mathcal{U}^\perp$, respectively.

Since $\overrightarrow{QP} = \boldsymbol{P}_{\mathcal{U}}\overrightarrow{QP} + \boldsymbol{P}_{\mathcal{U}^\perp}\overrightarrow{QP} = (\boldsymbol{P}_{\mathcal{U}} + \boldsymbol{P}_{\mathcal{U}^\perp})\overrightarrow{QP}$ for every point P, Eq. (1.10) holds, where $\boldsymbol{I}$ is the identity matrix[3]. Hence, the identity matrix $\boldsymbol{I}$ is decomposed into the sum of the projection matrix onto the subspace $\mathcal{U}$ and the projection matrix onto its orthogonal complement $\mathcal{U}^\perp$ in the

[2] It is formally called "orthogonal projection", but we call it simply "projection", since we do not consider other types of projection in this book.

[3] Mathematicians often write it as $\boldsymbol{E}$, the initial of the German word Einheit ("unit"), or $\boldsymbol{U}$, the initial of "unit" and calle it the "unit matrix". Physicists and engineers usually write $\boldsymbol{I}$, the initial of "identity", and call it the "identity matrix".

form of Eq. (1.11). Note that the identity matrix itself is the projection matrix onto the entire space $\mathcal{R}^n$.

Since the vector $\overrightarrow{OQ} = \boldsymbol{P}_{\mathcal{U}}\overrightarrow{OP}$ on the right side of Eq. (1.5) and the vector $\overrightarrow{QP} = \boldsymbol{P}_{\mathcal{U}^\perp}\overrightarrow{OP}$ are orthogonal to each other, we have $\|\overrightarrow{OP}\|^2 = \|\overrightarrow{OQ}\|^2 + \|\overrightarrow{QP}\|^2$. Hence, Eq. (1.12) holds for an arbitrary vector $\boldsymbol{x}$ (Fig. 1.5).

For the projection matrix $\boldsymbol{P}_{\mathcal{U}}$, Eqs. (1.13) and (1.14) hold [4](↪ Problem 1.3).

Equation (1.13) states that $\boldsymbol{P}_{\mathcal{U}}$ is a symmetric matrix, as is evident from the definition of Eq. (1.9). Equation (1.14) states that the projected point is unchanged if it is projected again, which is evident from the meaning of projection. A matrix for which Eq. (1.14) holds is said to be *idempotent*. It can be shown that a matrix that is symmetric and idempotent represents the projection matrix onto some subspace (↪ Problem 1.4).

1.4 Projection onto Lines and Planes

A line l starting from the origin O and extending in the direction of unit vector $\boldsymbol{u}$ is a one-dimensional subspace.. The projection matrix $\boldsymbol{P}_l$ onto the line l is given by Eq. (1.15). Hence, the projection of $\overrightarrow{OP}$ onto l is given by Eq. (1.16), where we write the inner product of vectors $\boldsymbol{a}$ and $\boldsymbol{b}$ as $\langle \boldsymbol{a}, \boldsymbol{b} \rangle$ $(= \boldsymbol{a}^\top \boldsymbol{b})$ (↪ Appendix A.2) . The right side of Eq. (1.16) is the vector lying on the line l with length $\langle \overrightarrow{OP}, \boldsymbol{u} \rangle$ (Fig. 1.6), signed so that it is positive in the direction of $\boldsymbol{u}$ and negative in the opposite direction. This signed length is called the *projected length*. Thus, we conclude that *the inner product with a unit vector is the projected length onto the line in that direction*.

A plane Π passing through the origin O having a unit vector $\boldsymbol{n}$ as its surface normal is an $(n-1)$-dimensional subspace (strictly speaking, it is a "hyperplane", but we call it simply a "plane" if confusion does not occure). The line along the surface normal $\boldsymbol{n}$ is the orthogonal complement to the plane Π. Hence, if $\boldsymbol{P}_{\boldsymbol{n}}$ is the projection matrix onto Π, Eqs. (1.10) and (1.11) imply Eq. (1.17). Hence, the projection of $\overrightarrow{OP}$ onto Π is given by Eq. (1.18) (Fig. 1.7).

1.5 Schimidt Orthogonalization

A set of mutually orthogonal unit vectors is said to be an *orthonormal system*. We can convert n given linear independent vectors $\boldsymbol{a}_1$, ..., $\boldsymbol{a}_n$ to an orthonormal system $\boldsymbol{u}_1$, ..., $\boldsymbol{u}_n$ as follows. First,

[4]Equation (1.14) is the defintion of the (not necessarily orthogonal) projection. The orthogonal projection is defined by adding Eq. (1.13) (↪ Footnote 2).

let $\boldsymbol{u}_1 = \boldsymbol{a}_1/\|\boldsymbol{a}_1\|$. From Eq. (1.17), the projection matrix onto the subspace orthogonal to $\boldsymbol{u}_1$, i.e., the orthogonal complement, is $\boldsymbol{I} - \boldsymbol{u}_1\boldsymbol{u}_1^\top$. Hence, the projection of $\boldsymbol{a}_2$ onto it is given by Eq. (1.19), which is orthogonal to $\boldsymbol{u}_1$. It follows that its normalization to unit norm $\boldsymbol{u}_2 = \boldsymbol{a}_2'/\|\boldsymbol{a}_2'\|$ is a unit vector orthogonal to $\boldsymbol{u}_1$.

By the same argument, the projection matrix onto the subspace orthogonal to $\boldsymbol{u}_1$ and $\boldsymbol{u}_2$, i.e., the orthogonal complement, is $\boldsymbol{I} - \boldsymbol{u}_1\boldsymbol{u}_1^\top - \boldsymbol{u}_2\boldsymbol{u}_2^\top$. Hence, the projection of $\boldsymbol{a}_3$ onto it is given by Eq. (1.20), which is orthogonal to both $\boldsymbol{u}_1$ and $\boldsymbol{u}_2$. It follows that its normalization to unit norm $\boldsymbol{u}_3 = \boldsymbol{a}_3'/\|\boldsymbol{a}_3'\|$ is a unit vector orthogonal to both $\boldsymbol{u}_1$ and $\boldsymbol{u}_2$. Repeating the same argument, we see that if we already have mutually orthogonal unit vectors $\boldsymbol{u}_1$, ..., $\boldsymbol{u}_{k-1}$, the projection matrix onto the subspace orthogonal to $\boldsymbol{u}_1$, ..., $\boldsymbol{u}_{k-1}$, i.e., the orthogonal complement, is $\boldsymbol{I} - \boldsymbol{u}_1\boldsymbol{u}_1^\top - \cdots - \boldsymbol{u}_{k-1}\boldsymbol{u}_{k-1}^\top$. Hence, the projection of $\boldsymbol{a}_k$ onto it is given by Eq. (1.21), which is orthogonal to all of $\boldsymbol{u}_1$, ..., $\boldsymbol{u}_{k-1}$. It follows that its normalization to unit norm $\boldsymbol{u}_k = \boldsymbol{a}_k'/\|\boldsymbol{a}_k'\|$ is a unit vector orthogonal to all of $\boldsymbol{u}_1$, ..., $\boldsymbol{u}_2$. Repeating this for $k = 1$, ..., n, we obtain an orthonormal system $\boldsymbol{u}_1$, ..., $\boldsymbol{u}_n$. This procedure is called the *(Gram–)Schimidt orthogonalization*.

Problems of Chapter 1

1.1. (1) For an m-dimensional vector $\boldsymbol{a} = \left(a_i\right)$ and an n-dimensional vector $\boldsymbol{b} = \left(b_i\right)$, which denote vectors whose ith components are a_i and b_i, respectively, show that Eq. (1.19) holds, where the right side designates the $m \times n$ matrix whose (i, j) element is $a_i b_j$.

(2) Show that Eq. (1.20) holds, where tr denotes the trace of the matrix.

1.2. Express a point Q of subspace $\mathcal{U}$ in terms of the basis of $\mathcal{U}$, and differentiate the square norm from point P to show that the closest point of $\mathcal{U}$ from P is its projection Q.

1.3. Show that Eqs. (1.13) and (1.14) hold, using Eq. (1.9).

1.4* Show that a symmetric and idempotent matrix $\boldsymbol{P}$ is the projection matrix onto some subspace.

Chapter 2

Eigenvalues and Spectral Decomposition

2.1 Eigenvalues and Eigenvectors

For an $n \times n$ symmetric matrix, there exist n real numbers λ, called the *eigenvalues*, and n nonzero vectors $\boldsymbol{u}$, dalled the *eigenvectors*, such that Eq. (2.1) holds ($\hookrightarrow$ Appendix A.9). The n eigenvalues λ_1, ..., λ_n, which may include overlaps, are given as the solution of the nth degree equation of Eq. (2.2), called the *characteristic equation*, where $\boldsymbol{I}$ is the $n \times n$ identity matrix, and $|\cdots|$ denotes the determinant. The nth degree polynomial $\phi(\lambda)$ is called the *characteristic polynomial*. The n eigenvectors $\{\boldsymbol{u}_i\}$, $i = 1$, ..., n, can be chosen as an orthonormal system.

However, we need not actually solve the characteristic equation to obtain eigenvalues and eigenvectors. Various software tools which allow us to compute them with high accuracy and high speed using iterations are available, including the *Jacobi method* and the *Householder method*.

2.2 Spectral Decomposition

Let λ_1, ..., λ_n be the eigenvalues of $\boldsymbol{A}$, and $\{\boldsymbol{u}_i\}$, $i = 1$, ..., n, the corresponding orthonormal system of its eigenvectors, which defines an orthonormal basis of $\mathcal{R}$. Eq, (2.1) implies that $\boldsymbol{A}$ mapps the orthonormal basis vectors $\{\boldsymbol{u}_i\}$ of $\mathcal{R}^n$ to $\lambda_1\boldsymbol{u}_1$, ..., $\lambda_n\boldsymbol{u}_n$, respectively. Hence, From Eq. (1.1) the matrix $\boldsymbol{A}$ is written in the form of Eq. (2.3). In other words, *a symmetric matrix can be expressed in terms of its eigenvalues and eigenvectors*. This is called the *spectral decomposition*, or sometimes *eigenvalue decompositon*.

Since each term $\boldsymbol{u}_i\boldsymbol{u}_i^\top$ of Eq. (2.3) is the projection matrix onto the direction, called the *prin-*

cipal axis, of each eigenvector $\boldsymbol{u}_i$. ($\hookrightarrow$ Eq. (1.15)), Eq. (2.3) expresses the matrix $\boldsymbol{A}$ as a linear combination of the projection matrices onto the principal axes. In other words, the transformation of the space by a symmetric matrix is interpreted to be projections of each point onto the principal axes directions, followed by multiplication by the respective eigenvalues, which are then summed over all the principal axes.

The identity matrix $\boldsymbol{I}$ maps any orthonormal basis $\{\boldsymbol{u}_i\}$, $i = 1, ..., n$ to itself, i.e., $\boldsymbol{I}\boldsymbol{u}_i = \boldsymbol{u}_i$, hence all eigenvalues are 1, meaning that it has the spectral decomposition in the form of Eq. (2.4).

2.3 Rank

The number of linearly independent vectors among the n columns of matrix $\boldsymbol{A}$, or the number of linearly independent vectors among its n rows, is called the *rank* of that matrix.

Consider an arbitrary linear combination of the columns $\boldsymbol{a}_1, ..., \boldsymbol{a}_n$ of $\boldsymbol{A}$, which has the form of Eq. (2.5), where we let $\boldsymbol{c} = \begin{pmatrix} c_i \end{pmatrix}$. If r of the n eigenvalues are nonzero, we can let $\lambda_{r+1} = \cdots = \lambda_n = 0$ in Eq. (2.3) and write it as Eq. (2.6). This means that an arbitrary linear combination of the columns of $\boldsymbol{A}$ is written as a linear combination of mutually orthogonal, hence linearly independent, r vectors $\boldsymbol{u}_1, ..., \boldsymbol{u}_r$ ($\hookrightarrow$ Problem 2.1). Hence, the subspace spanned by $\boldsymbol{a}_1, ..., \boldsymbol{a}_n$ has dimension r, meaning that only r of the n columns are linearly independent. Thus, *the rank r of matrix $\boldsymbol{A}$ equals the number of its nonzero eigenvalues*. Since $\boldsymbol{A}$ is a symmetric matrix, this also holds for the rows, i.e., only r of the n rows are linearly independent.

2.4 Diagonalization of Symmetric Matrices

Equation (2.3) is rewritten as Eq. (2.7) ($\hookrightarrow$ Problem 2.2), where the matrix $\boldsymbol{U}$ of Eq. (2.8) is an *orthogonal matrix*, i.e., a matrix whose columns are an orthonormal system, consisting of columnas $\boldsymbol{u}_1, ..., \boldsymbol{u}_n$, for which Eq. (2.9) holds ($\hookrightarrow$ Problem 2.3). If $\boldsymbol{U}$ is an orthogonal matrix, so is its transpose $\boldsymbol{U}^\top$ ($\hookrightarrow$ Problem 2.4). Hence, the rows of an orthogonal matrix are also an orthonormal system. Multiplying Eq. (2.7) by $\boldsymbol{U}^\top$ from left and $\boldsymbol{U}$ from right on both sides, we obtain from Eq. (2.9) the equality of Eq. (2.10). Namely, *a symmetric matrix is transformed, if multiplied by a matrix consisting of its eigenvectors as columns from right and its transpose from left, to a diagonal matrix whose diagonal elements are the eigenvalues*. This is called the *diagonalization* of a symmetric matrix.

2.5 Inverse and Powers

If $\boldsymbol{A}$ is a *nonsingular matrix*, i.e., a matrix whose eigenvalues are all nonzero[1], or whose rank is n, it has its inverse $\boldsymbol{A}^{-1}$. Multiplying Eq. (2.1) by $\boldsymbol{A}^{-1}$ on both sides, we obtain $\boldsymbol{u} = \lambda \boldsymbol{A}^{-1}\boldsymbol{u}$, or $\boldsymbol{A}^{-1}\boldsymbol{u} = (1/\lambda)\boldsymbol{u}$. Hence, $\boldsymbol{A}^{-1}$ has the same eigenvectors as $\boldsymbol{A}$ with eigenvalues $1/\lambda$. Hence $\boldsymbol{A}^{-1}$ has the spectral decomposition of Eq. (2.11) ($\hookrightarrow$ Problem 2.5). As in the same way as Eqs. (2.7) and (2.10), we obtain the relationships of Eq. (2.12).

From Eq. (2.1), we see that $\boldsymbol{A}^2\boldsymbol{u} = \lambda\boldsymbol{A}\boldsymbol{u} = \lambda^2\boldsymbol{u}$, $\boldsymbol{A}^3\boldsymbol{u} = \lambda^2\boldsymbol{A}\boldsymbol{u} = \lambda^3\boldsymbol{u}$, ... , so that $\boldsymbol{A}^N\boldsymbol{u} = \lambda^N\boldsymbol{u}$. Hence, for an arbitrary natural number N, the matrix $\boldsymbol{A}^N$ has the same eigenvectors as $\boldsymbol{A}$ with eigenvalues λ^N. It follows that it has the spectral decomposition of Eq. (2.13). From this, we obtain, as in the case of Eq. (2.12), the expressions of Eq. (2.14). It is easy to see that this also applies to an arbitrary polynomial $f(x)$ so that we obtain Eqs. (2.15) and (2.16). These equations can be extend to an arbitrary function $f(x)$ for which its power series expansion converges. Further more, for any function $f(x)$ for which $f(\lambda_i)$, $i = 1, ..., n$ is defined, we can define $f(\boldsymbol{A})$ via Eq. (2.15). For example, if all the eigenvalues of $\boldsymbol{A}$ is nonnegative (such a matrix is said to be *positive semidefinite*; it is *positive definite* if al the eigenvalues are positive), its "square root" $\sqrt{\boldsymbol{A}}$ is defined by Eqs. (2.17) and (2.18) ($\hookrightarrow$ Problem 2.6).

We can view Eqs. (2.4) and (2.11) as special cases of Eq. (2.13) with $N = 0, -1$, where we define $\boldsymbol{A}^0 = \boldsymbol{I}$. For a nonsingular matrix $\boldsymbol{A}$, we can write $\boldsymbol{A}^{-N} = (\boldsymbol{A}^{-1})^N$ $(= (\boldsymbol{A}^N)^{-1})$ for a natural number N ($\hookrightarrow$ Problem 2.7). Then, we can see by combining Eqs. (2.11) and (2.13) that Eq. (2.13) holds for an arbitrary integer N. If $\boldsymbol{A}$ is a positive definite symmetric matrix, N can be extended to an arbitrary real number.

Problems of Chapter 2

2.1. Show that mutually orthogonal nonzero vectors $\boldsymbol{u}_1$, ..., $\boldsymbol{u}_m$ are linearly independent.

2.2. Show that Eq. (2.19) holds for n-dimensional vectors $\boldsymbol{a}_1$, ..., $\boldsymbol{a}_m$ and $\boldsymbol{b}_1$, ..., $\boldsymbol{b}_m$, where $\boldsymbol{A}$ and $\boldsymbol{B}$ are $n \times m$ matrices having columns $\boldsymbol{a}_1$, ..., $\boldsymbol{a}_m$ and columns $\boldsymbol{b}_1$, ..., $\boldsymbol{b}_m$, respectively.

2.3. Show that $\boldsymbol{U}$ is an orthogonal matrix, i.e., its columns form an orthonormal system, if and only if Eq. (2.9 holds.

[1] We can alternatively say that a matrix is nonsingular if its determinant (= the product of all the eigenvalues) is nonzero or if it has its inverse.

2.4. Show that if $\boldsymbol{U}$ is an orthogonal matrix, so is $\boldsymbol{U}^\top$, i.e., an orthogonal has not only orthonormal columns but also orthonormal rows.

2.5. Show that the matrix $\boldsymbol{A}$ of Eq. (2.3) and the matrix $\boldsymbol{A}^{-1}$ of Eq. (2.11) satisfy $\boldsymbol{A}^{-1}\boldsymbol{A} = \boldsymbol{I}$ by computing their product.

2.6. For the matrix $\sqrt{\boldsymbol{A}}$ defined by Eq. (2.17) or by the first equation of Eq. (2.18), show that $(\sqrt{\boldsymbol{A}})^2 = \boldsymbol{A}$ holds.

2.7. Show that for a nonsingular matrix $\boldsymbol{A}$, Eq. (2.20) holds for any natural number N.

Chapter 3

Singular Values and Singular Decomposition

3.1 Singular Values and Singular Vectors

For an $m \times n$ matrix $\boldsymbol{A}$ which is not the zero matrix $\boldsymbol{O}$, i.e., the matrix whose elements are all zero, we call a positive number σ (> 0) the *singular value*, an m-dimensional vector $\boldsymbol{u}$ $\boldsymbol{u}$ ($\neq \boldsymbol{0}$) the *left singular vector*, and an n-dimensional vector $\boldsymbol{v}$ ($\neq \boldsymbol{0}$) the *right singular vector* such that Eq. (3.1) hold. The left and right singular vectors are also simply called the *singular vectors*. There exist r set of such singular values and singular vectors, where r is the rank of the matrix $\boldsymbol{A}$, i.e. the number of linearly independent columns and the number of linearly independent rows (we discuss this shortly).

Multiplying the second equation of Eq. (3.1) by $\boldsymbol{A}$ from left on both sides, and multiplying the first equation by $\boldsymbol{A}^\top$ from left on both sides, we see that Eq. (3.2) holds. Namely, the left singular vector $\boldsymbol{u}$ is the eigenvector of the $m \times m$ symmetric matrix $\boldsymbol{A}\boldsymbol{A}^\top$, and the right singular vector $\boldsymbol{v}$ is the $n \times n$ symmetric matrix $\boldsymbol{A}^\top\boldsymbol{A}$. The squared singular value σ^2 is the eigenvalue of both of them. ($\hookrightarrow$ Problem 3.1). It is easy to see that $\boldsymbol{A}\boldsymbol{A}^\top$ and $\boldsymbol{A}^\top\boldsymbol{A}$ have a common positive eigenvalue σ^2 and that their eigenvectors $\boldsymbol{u}$ and $\boldsymbol{v}$ are related by Eq. (3.1) ($\hookrightarrow$ Problem 3.2).

Let $\sigma_1 \geq \cdots \geq \sigma_r$ (> 0) be the singular values of $\boldsymbol{A}$, where some of them may overlap. Since the corresponding r left singular vectors $\boldsymbol{u}_1$, ..., $\boldsymbol{u}_r$ and r right singular vectors are both eigenvectors of symmetric matrices, they can be chosen to form orthonormal systems.

For actually computing the singular values and singular vectors, we need not compute the eigenvalues and eigenvectors of $\boldsymbol{A}\boldsymbol{A}^\top$ and $\boldsymbol{A}^\top\boldsymbol{A}$. Various software tools that can compute them

with high speed and high accuracy are available. A typical one consists of transformation to a *bidiagonal matrix* by means of the Householder method and application of the *Golub-Reinsch method*.

3.2 Singular Value Decomposition

An $m \times n$ matrix $\boldsymbol{A}$ defines a linear mapping from the n-dimensional space $\mathcal{R}^n$ to the m-dimensional space $\mathcal{R}^m$ (*hookrightarrow* Appendix A.1). We can extend the orthonormal system $\boldsymbol{u}_1$, ..., $\boldsymbol{u}_r$ of the r left singular vectors to an orthonormal bais $\{\boldsymbol{u}_1, ..., \boldsymbol{u}_r, \boldsymbol{u}_{r+1}, ..., \boldsymbol{u}_m\}$ of $\mathcal{R}^m$. Similarly, we can extend the orthonormal system $\boldsymbol{v}_1$, ..., $\boldsymbol{v}_r$ of the r right singular vectors to an orthonormal basis $\{\boldsymbol{v}_1, ..., \boldsymbol{v}_r, \boldsymbol{v}_{r+1}, ..., \boldsymbol{v}_n\}$ of $\mathcal{R}^n$. From Eq. (3.2), these are eigenvectors of $\boldsymbol{A}\boldsymbol{A}^\top$ and $\boldsymbol{A}^\top\boldsymbol{A}$, and Eq. (3.3) holds: the eigenvalues for $\boldsymbol{u}_{r+1}$, ..., $\boldsymbol{u}_m$ and $\boldsymbol{v}_{r+1}$, ..., $\boldsymbol{v}_n$ are all 0. Hence, $\boldsymbol{A}\boldsymbol{v}_i = \boldsymbol{0}$, $i = r+1$, ..., n ($\hookrightarrow$ Problem 3.3(1)). This and the first equation of Eq. (3.1) means that $\boldsymbol{A}$ maps the orthonormal basis vectors $\{\boldsymbol{v}_1, ..., \boldsymbol{v}_n\}$ of $\mathcal{R}^n$ to $\sigma_1\boldsymbol{u}_1$, ..., $\sigma_r\boldsymbol{u}_r$, $\boldsymbol{0}$, ..., $\boldsymbol{0}$, respectively. Hence, from Eq. (1.1), we see tht $\boldsymbol{A}$ is expressed in the form of Eq. (3.4).

Similarly, we see that $\boldsymbol{A}^\top\boldsymbol{u}_i = \boldsymbol{0}$, $i = r+1$, ..., m ($\hookrightarrow$ Problem 3.3(2)), and this and the second equation of Eq. (3.1) means that $\boldsymbol{A}^\top$ maps the orthonormal basis vectors $\{\boldsymbol{u}_1, ..., \boldsymbol{u}_n\}$ of $\mathcal{R}^m$ to $\sigma_1\boldsymbol{v}_1$, ..., $\sigma_r\boldsymbol{v}_r$, $\boldsymbol{0}$, ..., $\boldsymbol{0}$, respectively. Hence, from Eq. (1.1), we see tht $\boldsymbol{A}^\top$ is expressed in the form of Eq. (3.5), which is the transpose of Eq. (3.4) on both sides. Thus, *an arbitrary matrix is expressed in terms of its singular values and singular vectors*. This is called the *singular value decomposition*.

3.3 Column Domain and Row Domain

Let $\mathcal{U}$ be the subspace spanned by the n columns of $\boldsymbol{A}$, and $\mathcal{V}$ the subspace spanned by its m rows. We call the the *column domain* and the *row domain*, respectively.

Consider an arbitrary linear combination of the columns $\boldsymbol{a}_1$, ..., $\boldsymbol{a}_n$ of $\boldsymbol{A}$, which has the form of Eq. (3.6), where we let $\boldsymbol{c} = \begin{pmatrix} c_i \end{pmatrix}$. From Eq. (3.4), this is rewritten as in Eq. (3.7). Namely, an arbitrary linear combination of the columns of $\boldsymbol{A}$ is a linear combination of mutually orthogonal, hence linearly independent ($\hookrightarrow$ Problem 2.4), vectors $\boldsymbol{u}_1$, ..., $\boldsymbol{u}_r$. Hence, the column domain $\mathcal{U}$ spanned by $\boldsymbol{a}_1$, ..., $\boldsymbol{a}_n$ is an r-dimensional subspace, for which $\boldsymbol{u}_1$, ..., $\boldsymbol{u}_r$ are an orthonormal basis. It follows that *only r columns are linearly independent*.

The rows of $\boldsymbol{A}$ are the columns of $\boldsymbol{A}^\top$. Hence, from Eq. (3.5) an arbitrary linear combination of rows is expressed as a linear combination of $\boldsymbol{v}_1$, ..., $\boldsymbol{v}_r$. Thus, the row domain $\mathcal{V}$ spanned by rows of $\boldsymbol{A}$ an r-dimensional subspace, for which $\boldsymbol{v}_1$, ..., $\boldsymbol{v}_r$ are an orthonormal basis. It follows that *only r rows are linearly independent*.

From these, we conclude that *the rank r of $\boldsymbol{A}$ equals the number of the singular values of $\boldsymbol{A}$* and that *the left singular vectors $\{\boldsymbol{u}_i\}$, i = 1, ..., r, and the right singular vectors $\{\boldsymbol{v}_i\}$, i = 1, ..., r, constitute the orthonormal basis of the columns domain $\mathcal{U}$ and the row domain $\mathcal{V}$, respectively*.

From Eq. (1.9), the projection matrix of $\mathcal{R}^m$ onto the column domain $\mathcal{U}$ and the projection matrix of $\mathcal{R}^n$ onto the row domain $\mathcal{V}$ are respectively given as in Eq. (3.8). Since each $\boldsymbol{u}_i$, $i = 1$, ..., r, is $\boldsymbol{u}_i \in \mathcal{U}$, we have $\boldsymbol{P}_{\mathcal{U}}\boldsymbol{u}_i = \boldsymbol{u}_i$. Hence, operation of $\boldsymbol{P}_{\mathcal{U}}$ to Eq. (3.4) from left does not cause any change. Similarly, we have $\boldsymbol{P}_{\mathcal{V}}\boldsymbol{v}_i = \boldsymbol{v}_i$ for the rows. Hence, $\boldsymbol{P}_{\mathcal{V}}$ to Eq. (3.4) from right does not cause any change. It follows that Eq. (3.9) hold.

3.4 Matrix Representation

As Eq. (2.7), Eq. (3.4) can be rewriten in the form of Eq. (3.10), where $\boldsymbol{U}$ and $\boldsymbol{V}$ are the matrices defined by Eq. (3.11), which are $m \times r$ and $n \times r$ matrices consisting of singular vectors $\boldsymbol{u}_1$, ..., $\boldsymbol{u}_r$ and $\boldsymbol{v}_1$, ..., $\boldsymbol{v}_r$ as columns, respectively. Rewriting Eq. (3.5) in the same way results in the transpose of Eq. (3.10) on both sides.

Since the r columns of the matrices $\boldsymbol{U}$ and $\boldsymbol{V}$ are orthonormal systems, we obtain Eq. (3.12) ($\hookrightarrow$ Problem 3.5), where the right sides are the $r \times r$ identity matrix. We also obtain Eq. (3.13) ($\hookrightarrow$ Problem 3.6).

Problems of Chapter 3

3.1. Show that for any matrix $\boldsymbol{A}$, the matrices $\boldsymbol{A}\boldsymbol{A}^\top$ and $\boldsymbol{A}^\top\boldsymbol{A}$ are both positive semidefinite symmetric matrices, i.e., symmetric matrices whose eigenvalues are all positive or zero.

3.2. Suppose one of the two matrices $\boldsymbol{A}\boldsymbol{A}^\top$ and $\boldsymbol{A}^\top\boldsymbol{A}$ has a positive eigenvalue σ for $\boldsymbol{A} \neq \boldsymbol{O}$. Show that it is also the eigenvalue of the other matrix and that their eigenvectors $\boldsymbol{u}$ and $\boldsymbol{v}$ are related by Eq. (3.1).

3.3. Show the following:

(1) If $\boldsymbol{A}\boldsymbol{A}^\top \boldsymbol{u} = \boldsymbol{0}$, then $\boldsymbol{A}^\top \boldsymbol{u} = \boldsymbol{0}$.

(2) If $\boldsymbol{A}^\top \boldsymbol{A}\boldsymbol{v} = \boldsymbol{0}$, then $\boldsymbol{A}\boldsymbol{v} = \boldsymbol{0}$.

3.4. Show that Eq. (3.12) holds.

3.5. Show that Eq. (3.13) holds.

Chapter 4

Pseudoinverse

4.1 Pseudoinverse

If an $m \times n$ matrix $\boldsymbol{A}$ ($\neq \boldsymbol{O}$) has the singular value decomposition in the form of Eq. (3.4), its *pseudoinverse*, or *generalized inverse*, of the *Moore-Penrose type* is defined to be the $n \times m$ matrix given by Eq. (4.1)[1]. If $\boldsymbol{A}$ is a nonsingular matrix, this coincides with the inverse $\boldsymbol{A}^{-1}$ of $\boldsymbol{A}$ ($\hookrightarrow$ Problem 4.1). In this sense, the pseudoinverse is a generalization of the inverse.

If we define the matrices $\boldsymbol{U}$ and $\boldsymbol{V}$ as in Eq. (4.6), Eq. (4.1) can be written, as Eq. (3.10) in the matrix form of Eq. (4.2).

4.2 Projection onto the Column and Row Domains

The inverse of a nonsingular matrix is defined so that the product is the identity matrix. However, the product of the pseudoinverse and the original matrix is note necessarily the identity. In fact, noting that $\{\boldsymbol{u}_i\}$ and $\{\boldsymbol{v}_i\}$, $i = 1, ..., r$, are orthonormal systems, we obtain from Eqs. (3.4) and (4.1), we obtain the relationships of Eq. (4.3) and (4.4) ($\hookrightarrow$ Eq. (3.8)), where we have noted that when the Kronecker delta δ_{ij} appears in summations $\sum$ over i or j (or both), only terms for which $i = j$ survive. From Eq. (4.3) and (4.4), we find that *the products* $\boldsymbol{A}\boldsymbol{A}^-$ *and* $\boldsymbol{A}^-\boldsymbol{A}$ *are the projection matrices onto the column domain* $\mathcal{U}$ *and the row domain* $\mathcal{V}$*, respectively* ($\hookrightarrow$ Problem 4.2).

Since the columns and rows of a nonsingular matrix are linearly independent, the columns and the rows both span the entire space, and the projection matrix onto the entire space is the identity matrix ($\hookrightarrow$ Eq. (1.11)). Hence, the pseudoinverse is a natural extension of the inverse.

[1] Pseudoinverses that are not of Moore-Penrose type can also be defined, but in this book we only consider pseudoinverses of Moore-Penrose type. Some authors write $\boldsymbol{A}^-$ for a "general" pseudoinverse and specifically write $\boldsymbol{A}^+$ for that of the Moore-Penrose type to make a distinction ($\hookrightarrow$ Footnote 2.

Since $\boldsymbol{P}_{\mathcal{U}}\boldsymbol{x} = \boldsymbol{x}$ for any $\boldsymbol{x} \in \mathcal{U}$, the matrix $\boldsymbol{P}_{\mathcal{U}}$ plays the role of the identity in the column domain $\mathcal{U}$. Hence, the first equation of Eq. (4.5) states that $\boldsymbol{A}^-$ *defines the inverse transformation of* $\boldsymbol{A}$ *in the column domain* $\mathcal{U}$. Similarly, since $\boldsymbol{P}_{\mathcal{V}}\boldsymbol{x} = \boldsymbol{x}$ for any $\boldsymbol{x} \in \mathcal{V}$, the matrix $\boldsymbol{P}_{\mathcal{U}}$ plays the role of the identity in the row domain $\mathcal{V}$. Hence, the second equation of Eq. (4.5) means that $\boldsymbol{A}^-$ *defines the inverse transformation of* $\boldsymbol{A}$ *in the row domain* $\mathcal{V}$.

For the projection matrices $\boldsymbol{P}_{\mathcal{U}}$ and $\boldsymbol{P}_{\mathcal{V}}$, the equalities $\boldsymbol{P}_{\mathcal{U}}\boldsymbol{u}_i = \boldsymbol{u}_i$ and $\boldsymbol{P}_{\mathcal{V}}\boldsymbol{v}_i = \boldsymbol{v}_i$ hold by definition. Hence, we obtain the identities of Eq. (4.6) for the pseudoinverse $\boldsymbol{A}^-$ in the same way as Eq. (3.9). From this observation, we obtain the fundamental identities of Eqs. (4.7) and (4.8) for the pseudoinvers[2]. Equation (4.7) is obtained by combining Eq. (4.4) and the first equation of Eq. (4.6). Alternatively, we may combine Eq. (4.3) and the second equation of Eq. (4.6). Equation (4.8) is, on the other hand, obtained by combining Eq. (4.3) and the first equation of Eq. (3.9). Alternatively, we may combine Eq. (4.4) and the second equation of Eq. (4.9). Equations (4.7) and (4.8) can also be obtained from the matrix representation of Eq. (4.2) ($\hookrightarrow$ Problem 4.3).

4.3 Pseudoinverse of Vectors

An n-dimensional vector $\boldsymbol{a}$ is an $n \times 1$ matrix, so it has its pseudoinverse. if $\boldsymbol{a} \neq \boldsymbol{0}$, its singular value decomposition is given by Eq. (4.9). The column domain is the one-dimensional space spanned by the unit vector $\boldsymbol{u} = \boldsymbol{a}/\|\boldsymbol{a}|$, and the row domain is $\mathcal{R}^1$ (= the set of real numbers) whose basis is 1. The singular value is $\|\boldsymbol{a}\|$. Hence, the pseudoinverse $\boldsymbol{a}^-$ is given by Eq. (4.10), i.e., *the transposed row vector divided by its square length* $\|\boldsymbol{a}\|^2$.

From Eqs. (3.4), (3.5), and (4.1), we see that $(\boldsymbol{A}^\top)^- = (\boldsymbol{A}^-)^\top$, which we simply write $\boldsymbol{A}^{-\top}$. Hence, the pseudoinverse of a row vector $\boldsymbol{a}^\top$ regarded as a 1×3 matrix is given by Eq. (4.11).

If we write the unit direction vector along vector $\boldsymbol{a}$ as $\boldsymbol{u} = \boldsymbol{a}/\|\boldsymbol{a}|$, the product of the pseudoinverse $\boldsymbol{a}^-$ and the vector $\boldsymbol{a}$ is given by Eq. (4.12), which is the projection matrix onto the direction of the vector $\boldsymbol{u}$. On the other hand, we see that Eq.(4.13) holds. Note that 1 (= the 1×1 identity matrix) is the projection matrix onto $\mathcal{R}^1$.

[2]The matrix $\boldsymbol{A}^-$ that satisfies Eq. (4.8) is the most *general* "pseudoinverse" of $\boldsymbol{A}$. By adding various conditions to this, we can define various (not necessarily of the Moor-Penrose type) pseudoinverse. If Eq. (4.7) is satisfied, it is said to be a "reflexive pseudoinverse". If $\boldsymbol{A}\boldsymbol{A}^-$ and $\boldsymbol{A}^-\boldsymbol{A}$ are both symmetric matrices, it is of the Moor-Penrose type./

4.4 Rank-constrained Pseudinverse

In Chapters 2 and 3, we pointed out that various software tools are available for vomputing eigenvalues, eigenvectors, and the singular value decomposition. However, this is not so for pseudoinverses. Basically, there is no software tool to automatically compute the pseudoinverse; if such a tool is offered, we should not use it. This is because all the computations that arise in physics and engineering are based of observation data obtained by measurement devices and sensors. Hence, all data contain noise to some extent. As a result, if we compute the singular value decomposition by Eq. (3.4), all the singular values σ_i are genrally positive. If some of σ_i are ideally 0 but are computed to be nonzero due to the noise, we may obtain unrealistic values using Eq. (4.1) due to $1/\sigma_i$.

Of course, this is not limited to pseudoinverses; it also applies to the computation of the usual inverses, e.g., when we use Eq. (2.11) to a matrix which is not really a nonsingular matrix. However, there is an important distinction: *while the inverse is defined only for nonsingular matrices, the pseudoinverse is defined for all nonzero matrices*. However, *we need to know the rank* for computing the pseudoinverse,using Eq. (4.1).

A simple way to judge the rank r of an $m \times n$ matrix $\boldsymbol{A}$ obtained from measurement data is to compute the singular value decomposition of Eq. (4.14) by letting $l = \min(m, n)$, and to find a value r such that Eq. (4.15) holds for the trailing singular values. Then, we regard them as noise and retain the singular values up to σ_r, i.e., we replace $\boldsymbol{A}$ by Eq. (4.16), truncating the trailing singular values, and compute its pseudoinverse $(\boldsymbol{A})_r^-$, which we calle the *rank-constrained pseudoinverse* (or *generalized inverse*). But how should we truncate the small singular values?

For a mathematical computation where the data are exact real numbers, possible errors are due to the rounding of finite length computation in the computer. Hence, we can use the smallest number that can be digitally represented in a computer, which is called the *machine epsilon*, as the threshold; some software tools are so designed. For computations of physics and engineering involving observation data, however, it is generally difficult to estimate the error magnitude; the estimation must done differently for different problems.

However, most application problems of physics and engineering are derived from some fundamental principles or laws. Hence, it is usually possible to do theoretical analysis based on such principles or laws to predict the rank r in an ideal case where the measurement devices or sensors

are assumed to be noiseless. Then, we can use the theoretical rank r regardless of the magnitude of the singular values to be truncated and compute the rank-constrained pseudoinverse of Eq. (4.16).

We are then interested in estimating the difference between the rank-constrained matrix obtained by truncating the trailing singular values and the original matrix. This is measured by the matrix norm.

4.5 Evaluation by Matrix Norm

The *matrix norm* of an $m \times n$ matrix $\boldsymbol{A} = \Big(A_{ij}\Big)$ is defined by Eq. (4.17). This is called the *Frobenius norm* or the *Euclid norm*, for which Eq. (4.18) holds, where tr denotes the matrix trace. In face, the three terms of Eq. (4.18) are all equal to $\sum_{i=1}^{m} \sum_{j=1}^{n} A_{ij}^2$ from the definition ($\hookrightarrow$ Problems 4.4 and 4.5).

Using Eq. (4.18), we can evaluate the difference between the matrix $\boldsymbol{A}$ of Eq. (4.14) and the matrix $(\boldsymbol{A})_r$ of Eq. (4.16), measured in the square matrix norm, as shown in Eq. (4..19), where we note that $\mathrm{tr}(\boldsymbol{v}_i \boldsymbol{v}_i^\top) = \|\boldsymbol{v}_i\|^2 = 1$ from Eq. (1.20). Thus, we conclude that the difference between the matrix $\boldsymbol{A}$ and the matrix $(\boldsymbol{A})_r$ obtained by truncating singular values is equal to *the square sum of the truncated singular values*[3]. Namely, Eq. (4.20) holds. This can be also derived using the matrix representation ($\hookrightarrow$ Problem 4.6).

Problems of Chapter 4

4.1. Show that if $\boldsymbol{A}$ is nonsingular, i.e., $m = n$ and its eigenvalues are all nonzero, or $r = n$, Eq. (4.1) defines the inverse $\boldsymbol{A}^{-1}$ of $\boldsymbol{A}$.

4.2. Using Eqs. (3.10) and (4.2), show that Eq. (4.5) holds.

4.3. Using Eqs. (3.10) and (4.2), show that Eq. (4.7) holds.

4.4. Show that Eq. (4.21) holds for the matrix trace, where the sizes of the matrices are such that the products can be defined.

4.5. Show that Eq. (4.22) holds for orthogonal matrices $\boldsymbol{U}$ and $\boldsymbol{V}$ having sizes such that the products can be defined.

[3]It can be shown that for a given matrix $\boldsymbol{A}$, the matrix $\boldsymbol{A}'$ of the same size that minimizes $\|\boldsymbol{A} - \boldsymbol{A}'\|$ subject to the constraint $\mathrm{rank}(\boldsymbol{A}') = r$ is given by $\boldsymbol{A}' = (\boldsymbol{A})_r$ [3]. The proof is rather complicated.

4.6. Show that if matrix $\boldsymbol{A}$ has a singular value decomposition in the form of Eq. (3.10), its norm is given by Eq. (4.23) so that Eq. (4.20) is obtained.

Chapter 5

Least-squares Solution of Linear Equations

5.1 Linear Equations and Least Squares

Consider m simultaneous linear equations of n variables x_1, ..., x_n in the form of Eq. (5.1). Using vectors and matrices, We can write them in the vector and matrix form of Eq. (5.2), where we the $m \times n$ matrix $\boldsymbol{A}$, n-dimensional vector$\boldsymbol{x}$, and the m-dimensional vector $\boldsymbol{b}$ are defined by Eq. (5.3). In the following, we assume that $\boldsymbol{A} \neq \boldsymbol{O}$.

As is well known, Eq. (5.2) has a unique solution if and only when $n = m$ and when the determinant of $\boldsymbol{A}$ is nonzero, i.e., wheh $\boldsymbol{A}$ is nonsingular. In that case, the best known procedure for manually computing the solution is the *Gaussian elimination*, and the mathematically equivalent programm package called the *LU-decomposition* is available. In many physic and engineering applications that involve observation data, however, problems with $n \neq m$ frequently occur.

Each equation of Eq. (5.1) is interpreted to be a measurement process for estimating the n parameters x_1, ..., x_n. Theoretically, we only need n measurements for determining n parameters. However, we often repeat the measurement m ($> n$) times, considering that the observations may contain noise. In some cases, there are some constraints which allows measurement only m ($< n$) times. In such cases for which $n \neq m$, a practical method for estimating x_1, ..., x_n is to compute their values that satisfy all the equations of Eq. (5.1) sufficiently well "as a whole". A typical strategy for this is to minimize the sum of the squares of the differences between the right and left sides the individual equations. Namely, we compute x_1, ..., x_n that minimize Eq. (5.4). This is called the *least-squares method*. The value J of Eq. (5.4) is called the *residual sum of squares* or,

for short, the *residual*. If we write Eq. (5.1) in the form of Eq. (5.2) using vectors and matrices, the residual J of Eq. (5.4) is written as Eq. (5.5).

However, the value of $\boldsymbol{x}$ that minimize J may not be determined uniquely if we cannot repeat the observation a sufficient number of times. In that case, we choose from among multiple possibilities the value $\boldsymbol{x}$ that minimizes $\|\boldsymbol{x}\|^2$. This reflects the fact that in many physics and engineering problems the value $\|\boldsymbol{x}\|^2$ represents some physical quantity that, like heat generation or required energy, should desirably be as small as possible. In view of this, we call the value $\boldsymbol{x}$ for which (i) the residual J is minimized and (ii) $|\boldsymbol{x}\|^2$ is minimum the *least-squares solution*.

The least-squares method was introduced by the German mathematician Karl Gauss (1777–1855) for computing the motion of planets from telescope observation data. He also introduced various numerical techniques for computing simultaneous linear equations and integrations accurately and efficiently, which are now the foundations of today's numerical analysis. In order to justify his least-squares method, he established a mathematical model of numerical noise contained in observation data. Asserting that such a noise distribution is the most "normal", he called it the model the *normal distribution* (see Sec. 6.2 of the next chapter). It plays the fundamental role in today's statistical analysis. On the other hand, physicists and engineers often call it the *Gaussian distribution* in honor of Gauss. He also made many contribution in pure mathematics, including the fundamental theorem of algebra (the Gauss theorem). At the same time, he also established many differential and integral formulas of electromagnetics and fluid dynamics, which are the basis of today's physics.

5.2 Computing the Least-squares Solution

In general, the solution that minimizes Eq. (5.5) is obtained by differentiating J by $\boldsymbol{x}$, letting the result be $\boldsymbol{0}$, and solving the resulting equation $\nabla_{\boldsymbol{x}} J = \boldsymbol{0}$, which is called the *normal equation*. However, the solution has different forms, depending on whether $m > n$ or $m < n$ and whether $r = n$, $r = m$, or otherwise (Problems 5.1– 5.4). Here, we show that the most general form of the least-square solution that encompasses all the cases is obtained, using the projection matrix and the pseudoinverse, without involving differentiation or solving the normal equation.

Let $\mathcal{U}$ be the column domain of $\boldsymbol{A}$ of Eq. (5.3), i.e., the space spanned by the columns of $\boldsymbol{A}$. This is a subspace of $\mathcal{R}^m$. From Eq. (1.12), we can express the square norm of a vector as the

sum of the square norm onto subspace $\mathcal{U}$ and the square norm of the rejection from it, i.e., the projection onto the orthogonal complement $\mathcal{U}^\perp$. Hence, the residual J of Eq. (5.5) can be written as Eq. (5.6). Here, we note that $\boldsymbol{P}_{\mathcal{U}}\boldsymbol{A}\boldsymbol{x} = \boldsymbol{A}\boldsymbol{x}$ and $\boldsymbol{P}_{\mathcal{U}^\perp}\boldsymbol{A}\boldsymbol{x} = \boldsymbol{0}$ hold because $\boldsymbol{A}\boldsymbol{x}$ is a linear combination of the columns of $\boldsymbol{A}$ and is included in the column domain $\mathcal{U}$. Since the last term of Eq. (5.6) does not contain $\boldsymbol{x}$, the least-squares solution satisfied Eq. (5.7).

This is interpreted as follows. Since $\boldsymbol{A}\boldsymbol{x} \in \mathcal{U}$, Eq. (5.2) evidently has no solution unless $\boldsymbol{b} \in \mathcal{U}$. Hence, *we replace the vector* $\boldsymbol{b}$ *by its projection* $\boldsymbol{P}_{\mathcal{U}}\boldsymbol{b}$ *onto* $\mathcal{U}$. Since the part of $\boldsymbol{b}$ that is outside the column domain $\mathcal{U}$ is $\boldsymbol{P}_{\mathcal{U}^\perp}\boldsymbol{b}$, the residual equals $\|\boldsymbol{P}_{\mathcal{U}^\perp}\boldsymbol{b}\|^2$ (Fig. 5.1).

We are assuming that $\boldsymbol{A} \neq \boldsymbol{O}$, so $\boldsymbol{A}$ has the singular value decomposition of the form of Eq. (3.4). The left side of the first equation of Eq. (5.7) is rewritten in the form of Eq. (5.8). From the expression of $\boldsymbol{P}$ of Eq. (3.8), the right side is rewritten in the form of Eq. (5.9). Since Eqs. (5.8) and (5.8) are expansions in terms of the orthonormal system $\{\boldsymbol{u}_i\}$ ($\hookrightarrow$ Appendix A.7), we have $\sigma_i\langle \boldsymbol{v}_i, \boldsymbol{x}\rangle = \langle \boldsymbol{u}_i, \boldsymbol{b}\rangle$ and hence Eq. (5.10). If we extend the n-dimensional vectors $\boldsymbol{v}_1$, ..., $\boldsymbol{v}_r$ to make an orthonormal basis $\{\boldsymbol{v}_1, ..., \boldsymbol{v}_r, \boldsymbol{v}_{r+1}, ..., \boldsymbol{v}_n\}$ of $\mathcal{R}^n$, we can expand $\boldsymbol{x}$ with respect to this basis in the form of Eq. (5.11) ($\hookrightarrow$ Appendix Eq. (A.35)). However, $\langle \boldsymbol{v}_{r+1}, \boldsymbol{x}\rangle$, ..., $\langle \boldsymbol{v}_n, \boldsymbol{x}\rangle$ are unknown.

Following the principle that we choose the solution that minimizes Eq. (5.11), we adopt the solution for which $\langle \boldsymbol{v}_{r+1}, \boldsymbol{x}\rangle = \cdots = \langle \boldsymbol{v}_n, \boldsymbol{x}\rangle = 0$ ($\hookrightarrow$ Appendix Eq. (A.36)). As a result, $\boldsymbol{x}$ is expressed as Eq. (5.13). Namely, the least-squares solution $\boldsymbol{x}$ is given by Eq. (5.14).

Note that, as pointed out in the preceding chapter, we need to know the rank r of $\boldsymbol{A}$ for computing $\boldsymbol{A}^-$. It should be estimated from the fundamental principles or the fundamental laws behind the problem in question by inferring what the rank will be if the observation data are ideal. If no theoretical relationships or constraints among the n variables and m equations o Eq. (5.1), we can let $r = \min(n, m)$. Otherwise, we compute the rank-constrained pseudoinvers, using the estimated rank r.

5.3 Multiple Equations of One Variable

Consider, as an example, the simultaneous linear equaions of Eq. (5.15) for $n = 1$, where we assume that a_1, ..., a_m are not all 0. In vector form, it is written as Eq. (5.16). Since the pseudoinverse $\boldsymbol{a}^-$ of vector $\boldsymbol{a}$ is given by Eq. (4.10), the least-squares solution is given by Eq. (5.17). Formally, it is rewritten in the form of Eq. (5.18), where terms for $x = b_i/a_i$ are ignored. This is interpreted to

be the weighted average of the individual solutions $x = b_i/a_i$ of Eq. (5.15) with weights a_i^2. It can be easily shown that this is the solution that minimizes the residual J of Eq. (5.19) ($\hookrightarrow$ Problem 5.5).

5.4 Single Multivariate Equation

For another example, consider a single linear equation of Eq. (5.20), where we assume that a_1, ..., a_n are not all 0. In vector form, it is written as Eq. (5.21). Since this is rewritten as $\boldsymbol{a}^\top \boldsymbol{x} = b$, the least-squares solution if given by $(\boldsymbol{a}^\top)^- \boldsymbol{x}$. A row vector $\boldsymbol{a}^\top$ has its pseudoinverse $\boldsymbol{a}^{-\top}$ $(= (\boldsymbol{a}^\top)^- = (\boldsymbol{a}^-)^\top)$ in the form of Eq. (4.11). Hence, the least-squares solution is given by Eq. (5.22). It is easy to see that $\langle \boldsymbol{a}, \boldsymbol{x} \rangle = b$ holds. Since the ith component of Eq. (5.22) is $x_i = ba_i/\|\boldsymbol{a}\|^2$, we can write the ith term on the left side of Eq. (5.20) is given by Eq. (5.23). This means that the n terms on the left side of Eq. (5.20) are portions of b on the right side distributed in proportion to the ratio$a_i^2 : \cdots : a_n^2$. It is easy to confirm that Eq. (5.22) is the solution that minimizes $\|\boldsymbol{x}\|^2$ subject to the condition that $\boldsymbol{x}$ satisfies Eq. (5.20) ($\hookrightarrow$ Problem 5.6).

Problems of Chapter 5

5.1. Show that if $m > n$ and if the columns of $\boldsymbol{A}$ are linearly independent, i.e., $r = n$, then

(1) the least-squares solution $\boldsymbol{x}$ is given by Eq. (5.24) and

(2) the residual J is written in the form of Eq. (5.25).

5.2. Show that if $m > n = r$, Eq. (5.26) holds.

5.3. Show that if $n > m$ and if the rows of $\boldsymbol{A}$ are linearly independent, i.e., $r = m$, then the residual J is 0 and the least-squares solution $\boldsymbol{x}$ is given by Eq. (5.27).

5.4. Show that if $n > m = r$, Eq. (5.28) holds.

5.5. Show that the solution x given by Eq. (5.17) minimizes the sum of square of Eq. (5.19).

5.6. Show that Eq. (5.22) minimizes $\|\boldsymbol{x}\|^2$ over all $\boldsymbol{x}$ that satisfy Eq. (5.20).

Chapter 6

Probability Distribution of Vectors

6.1 Covariance Matrices of Errors

A vector $\boldsymbol{x}$ is said to be a *random variable* if its value is not deterministic but is specified by some (or assumed) *probability distribution*. In physics and engineering, we often regard the values obtained by measurement devices and sensors as random variables. Usually, an observed value $\boldsymbol{x}$ is interpreted to be the sum of its true value $\bar{\boldsymbol{x}}$ (a definitive value) and some noise term $\Delta\boldsymbol{x}$ (a random variable) in the form of Eq. (6.1). We usually assume that the noise term $\Delta\boldsymbol{x}$ has *expectation*, or average, $\boldsymbol{0}$; if it has an expectation not equal to $\boldsymbol{0}$, we can model its probability distribution after subtracting it. Namely we assume that Eq. (6.1) holds, where $E[\,\cdot\,]$ denotes expectation with respect to the probability distribution of the noise. We define the *covariance matrix* of the noise by Eq. (6.2) ($\hookrightarrow$ Problem 6.1). From this definition, we see that $\boldsymbol{\Sigma}$ is a positive semidefinite matrix, i.e., its eigenvalues are positive or zero ($\hookrightarrow$ Problem 6.2). From Eq. (6.3), the *mean square* of the noise term $\Delta\boldsymbol{x}$ is given by Eq. (6.3), i.e., the trace of the covariance matrix $\boldsymbol{\Sigma}$ ($\hookrightarrow$ Problem 6.3).

Let σ_1^2, ..., σ_n^2 be the nonnegative eigenvalues of the covariance matrix $\boldsymbol{\Sigma}$, and σ_1^2, ..., σ_n^2 the orthonormal system of the corresponding unit eigenvectors. Then, $\boldsymbol{\Sigma}$ has the spectral decomposition in the form of Eq. (6.5). We call the directions of the vectors $\boldsymbol{u}_1$, ..., $\boldsymbol{u}_n$ the *principal axes* of the noise distribution. The values σ_1^2, ..., σ_n^2 indicate the variance of the noise in the respective directions, i.e., σ_1, ..., σ_n are their standard deviations. In fact, the magnitude of the noise term $\Delta\boldsymbol{x}$ along $\boldsymbol{u}_i$, i.e., the projected length in the direction of $\boldsymbol{u}_i$ is given by $\langle \Delta\boldsymbol{x}, \boldsymbol{u}_i \rangle$, as shown in Eq. (1.16), and its mean square is given by Eq. (6.6). If all the eigenvalues are equal, i.e., if $\sigma_1^2 = \cdots = \sigma_n^2$ $(= \sigma^2)$, the noise is said to be *isotropic*, in which case the noise occurence is equally likely in any direction and the covariance matrix $\boldsymbol{\Sigma}$ of Eq. (6.3) ahs the form of Eq. (6.7). $\hookrightarrow$ Eq. (2.4)).

Otherwise, the noise is said to be *anisotropic*, in which case the likelihood of the occurence of $\boldsymbol{x}$ depends on the direction. In particular, the the eigenvector $\boldsymbol{u}_{\max}$ for the maximum eigenvalue $\sigma_{\max}^2$ indicate the direction along which the noise is most likely to occur, and $\sigma_{\max}^2$ is the variance in that direction. This is because the projected length of the noise term $\Delta\boldsymbol{x}$ onto the direction of a unit vector $\boldsymbol{u}$ is given by $\langle \Delta\boldsymbol{x}, \boldsymbol{u}\rangle$ ($\hookrightarrow$ Sec. 1.4), and its square means is, as shown in Eq. (6.6), $E[\langle \Delta\boldsymbol{x}, \boldsymbol{u}\rangle^2] = \langle \boldsymbol{u}, \boldsymbol{\Sigma}\boldsymbol{u}\rangle$, which is a quadratic form of the symmetric matrix $\boldsymbol{\Sigma}$. Hence, the unit vector $\boldsymbol{u}$ that maximize it is given by the unit eigenvector $\boldsymbol{u}_{\max}$ for the maximum eigenvalue $\sigma_{\max}$ ($\hookrightarrow$ Appendix A.10).

If there exists an eigenvector $\boldsymbol{u}_i$ for which the eigenvalue is 0, we infer that no noise occurs in that direction. In practice, this means that the variation of $\boldsymbol{x}$ in that direction is physically prohibited.

6.2 Normal Distribution of Vectors

A typical probability distribution is the *normal distribution*. In the n-dimensional space $\mathcal{R}^n$, it is specified by the expectation $\bar{\boldsymbol{x}}$ and the covariance matrix $\boldsymbol{\Sigma}$ alone. Its distribution density has the form of Eq. (6.8), where C is a normalization constant set so that the integration over the entire space $\mathcal{R}^n$ equals 1 (to be precise, it is $1/\sqrt{(2\pi)^n\sigma_1^2\cdots\sigma_n^2}$). The distribution extends to infinity, and the covariance matrix $\boldsymbol{\Sigma}$ is assumed to be positive definite (i.e., all the eigenvalues are positive). It satisfies the identities of Eq. (6.9), where $\int_{\mathcal{R}^n}(\cdots)d\boldsymbol{x}$ denotes integration over the entire $\mathcal{R}^n$.

If a surface on which the probability density $p(\boldsymbol{x})$ is constant has the form of Eq. (6.10), it is called the *error ellipsoid* (Fig. 6.1). This is an ellipsoid centered on $\bar{\boldsymbol{x}}$; it is also called the *error ellipse* for two variables and the *confidence interval* for a single variable. Each of the eigenvectors of the covariance matrix $\boldsymbol{\Sigma}$ is the axis symmetry, and the radius in that direction is the standard deviation σ_i in that direction ($\hookrightarrow$ Problems 6.4 and 6.5). Thus, the error ellipse visualizes directional dependence of the likelihood of error occurrence.

In some engineering applications, including computer graphics and computer vision, we often consider covariance matrices which are not positive definite. The fact that the covariance matrix has eigenvalue 0 means that the disturbance in the corresponding eigenvector is prohibited. Suppose, for example, we want to evaluate the uncertainty of the position of a particular point on the display surface or in the image. Then, the noise disturbance occurs only within a two-dimensional plane,

and the perpendicular displacement is prohibited. It seems then that it is sufficient to define a two-dimensional coordinate system in that plane and consider a normal distribution of two variables. However, it is often more appropriate to regard that plane as a surface in the three-dimensional space. This is because for such analysis, we define a particular point, called the *viewpoint*, in the three-dimensional scene, which corresponds to the position of the human eye or the camera lens center, and analyze the geometric properties of the figures on the display surface or in the image, which is identified with the camera image plane, by regarding them as a perspective view of the three-dimensional scene (Fig. 6.2).

Considering such applications, let r be the rank of the $n \times n$ covariance matrix $\boldsymbol{\Sigma}$, and $\boldsymbol{u}_1$, ..., $\boldsymbol{u}_r$ the orthonormal system of its unit eigenvectors for positive eigenvalues σ_1^2, ..., σ_r^2 (> 0). We denote the r-dimensional subspace they span by $\mathcal{U}$. In other words, we are assuming that all stochastic deviations occur within $\mathcal{U}$ and that no displacements are allowed in the direction of $\mathcal{U}^\perp$. In this case, the probability density of the normal distribution with expectation $\bar{\boldsymbol{x}}$ and covariance matrix $\boldsymbol{\Sigma}$ has the form of Eq. (6.11), where $\boldsymbol{\Sigma}^-$ is the pseudoinvers of the covariance matrix $\boldsymbol{\Sigma}$, and C is a normalization constant determined so that the integration over $\mathcal{U}$, not over the entire $\mathcal{R}^n$, equals 1 (to be precise, it is $1/\sqrt{(2\pi)^r \sigma_1^2 \cdots \sigma_r^2}$). Then, the relations of Eq. (6.12) hold, where $\int_{\mathcal{U}}(\cdots)d\boldsymbol{x}$ denotes integration over $\mathcal{U}$.

The covariance matrix $\boldsymbol{\Sigma}$ and its pseudoinverse $\boldsymbol{\Sigma}^-$ have the spectral decomposition in the form of Eq. (6.13). Hence, the projection matirx $\boldsymbol{P}_{\mathcal{U}}$ ($= \sum_{i=1}^r \boldsymbol{u}_i \boldsymbol{u}_i^\top$) onto the subspace $\mathcal{U}$ satisfies the relations of Eq. (6.14), and hence Eq. (6.15) holds ($\hookrightarrow$ Appendix Eq. (A.27)). In other words, the use of the pseudoinverse $\boldsymbol{\Sigma}^-$ means that we are considering the normal distribution not of $\boldsymbol{x} - \bar{\boldsymbol{x}}$ but of its projection $\boldsymbol{P}_{\mathcal{U}}(\boldsymbol{x} - \bar{\boldsymbol{x}})$ onto $\mathcal{U}$. Within $\mathcal{U}$, the distribution is regarded as a normal distribution with variance σ_i^2 (> 0) in each principal axis direction, defining a covariance matrix that is positive definite within $\mathcal{U}$.

Example. Normal distribution over the image plane

The normal distribution over the image plane is represented as follows. Let $(\bar{x}, \bar{y})$ be the true position of an observed point (x, y), and write $(x, y) = (\bar{x} + \Delta x, \bar{y} + \Delta y)$. We assume that the noise terms Δx and Δy are subject to a normal distribution with expectation is 0 having the variance/covariance given by Eq. (6.16). We regard the image plane, or the display surface, as the plane $z = 1$ in the three-dimensional space (Fig. 6.3). If we represent points (x, y) and $(\bar{x}, \bar{y})$

by three-dimensional vectors of Eq. (6.17)[1], the probability density of $\boldsymbol{x}$ is written in the form of Eq. (6.18), where the covariance matrix $\boldsymbol{\Sigma}$ has the form of Eq. (6.19).

6.3 Probability Distribution over a Sphere

Applications which involve non-positive definite covariance matrices, other than distributions over planes, include distributions over a "sphere". In some problems of physics and engineering, sensor data are directional, i.e., only orientations can be measured. If we normalize the direction vector to unit norm, an observed datum can be regarded as a point over a unit sphere.

A typical example is observation using images alone. A camera can identify the direction of incoming ray of light, but the depth, i.e., the distance to the object, is unknown. This is the case however many cameras are used. In fact, if we move the camera over a short distance relative to a small object nearby or over a long distance relative to a large object in the distance, the observed image is the same. Today, various computer vision techniques are established for reconstructing the shape of three-dimensional scenes and objects using camera images, the absolute scale of the reconstructed shape is indeterminate. This scale indeterminacy is not limited to the reconstructed shape. Many types of matrix that characterize the structure of the scene can be computed from images, but they are often determined up to scale[2]. Usually, such matrices are normalized so that the sum of the squares of the elements is 1. If we view an $n \times n$ matrix as an n^2-dimensional vector consisting of the n^2 matrix elements, it can be regarded as a point on a unit sphere in the n^2-dimensional space after normalization.

Considering these, we assume that the measured value $\boldsymbol{x}$ is an n-dimensional unit vector. It is identified with a point on the $(n-1)$-dimensional unit sphere S^{n-1} in the n-dimensional space $\mathcal{R}^n$, and a probability distribution is defined around its true position $\bar{\boldsymbol{x}}$. However, mathematical analysis is generally very difficult. First of all, the normal distribution, which is the most common distribution, cannot be defined, because the sphere S^{n-1} is of finite size while the normal distribution extends infinitely over the entire space $\mathcal{R}^n$. In practical problems, however, today's sensors including cameras are highly accurate so that the noise component $\Delta\boldsymbol{x}$ of $\boldsymbol{x}$ is usually very small[3].

[1] This is equivalent to representing a point in the plane by its "homogeneous coordinates" as done in projective geometry.

[2] Typical examples include matrices called the "fundamental matrix" and the "homography matrix".

[3] For example, the accuracy in locating a particular point in an image using an image processing algorithm is usually around 1∼3 pixels.

Consequently, the distribution of $\boldsymbol{x}$ is thought to be limited to a small region surrounding $\bar{\boldsymbol{x}}$ on the sphere S^{n-1}. Hence, we can view this as a distribution over the tangent plane to S^{n-1} at $\bar{\boldsymbol{x}}$ (Fig. 6.4). We can then define the expectation and the covariance matrix of $\boldsymbol{x}$ and hence the normal distribution of $\boldsymbol{x}$.

The tangent plane to S^{n-1} at $\bar{\boldsymbol{x}}$ is an $(n-1)$-dimensional (hyper-) plane, whose unit surface normal is $\bar{\boldsymbol{x}}$ itself. Hence, from Eq. (1.17) the projection matrix onto the tangent plane is given by Eq. (6.20). Consider, as a practical application, the reliability evaluation of the measurement $\boldsymbol{x}$. Suppose we repeat the measurement and observe $\boldsymbol{x}_1$, ..., $\boldsymbol{x}_N$ as the result. Or suppose you want to evaluate the performance of a computational procedure for computing $\boldsymbol{x}$. You artificially add random noise to the original observations and compute $\boldsymbol{x}$ from the noisy data. Let $\boldsymbol{x}_1$, ..., $\boldsymbol{x}_N$ the results for different noise. In either case, you want to evaluate how $\boldsymbol{x}_1$, ..., $\boldsymbol{x}_N$ differ from the theoretical value $\bar{\boldsymbol{x}}$.

Let $\boldsymbol{x}_\alpha \in S^{n-1}$ be the αth measurement. Its projection onto the tangent plane is given by Eq. (6.21) (Fig. 6.5). The *sample mean* $\boldsymbol{m}$ and the *sample covariance matrix* $\boldsymbol{S}$ are computed by Eq. (6.22), where the expression"sample $\cdots$" means replacing the integration in expectation computations, such as Eqs. (6.9) and (6.12), with respect to the true probability distribution by the arithmetic average over all "realizations", for which many different terms are used including observations, measurements, samples, and data.

The sample mean $\boldsymbol{m}$ indicates the averatge deviation from the true positio $\bar{\boldsymbol{x}}$ on the tangent plane. Its magnitude $\|\boldsymbol{m}\|$, which is ideally 0, is called the *bias*[4]. The diagonal element S_{ii} of the sample covariance matrix $\boldsymbol{S}$ is the samle variance of the ith component $\hat{x}_{i\alpha}$ of $\hat{\boldsymbol{x}}_\alpha$, and the non-diagonal element S_{ij}, $i \neq j$ is the sample covariance of $\hat{x}_{i\alpha}$ and $\hat{x}_{j\alpha}$ ($\hookrightarrow$ Problem 6.6)). The square root of the trace of the sample covariance matrix $\boldsymbol{S}$, given by Eq. (6.23) is called the *root-mean-square error*, or the *RMS error* for short, which is a typical indicator of the observation accuracy or computational performance.

From the definition of $\boldsymbol{P}_{\bar{\boldsymbol{x}}}$ of Eq. (6.21), the sample covariance matrix $\boldsymbol{S}$ satisfies Eq. (6.24) and has rank $n-1$. If the distribution of $\boldsymbol{x}$ is regarded as a normal distribution, its *empirical probability density* is given by Eq. (6.25), where C is the normalization constant determined so that integratio over the tangent plane is 1. The expression "empirical $\cdots$" means replacing the

[4]For a random variable, this term usually means the deviation of its expectation from the true value. If it is 0, the random variable is said to be "unbiased". For realizations, the bias means the deviation of the samle mean from its true value. Here, we are using this term in the realization sense.

parameters included in the theoretical expression by values estimated from realizations like the sample mean and the sample covariance matrix.

Problems of Chapter 6

6.1. Show that If we let $\boldsymbol{x} = \begin{pmatrix} x_i \end{pmatrix}$, the diagonal element Σ_{ii} of the covariance matrix $\boldsymbol{\Sigma}$ of Eq. (6.3) gives the variance of x_i and the non-diagonal element Σ_{ij}, $i \neq j$ gives the covariance of x_i and x_j.

6.2. Show that the matrix $\boldsymbol{X} = \boldsymbol{x}\boldsymbol{x}^\top$ defined from a vector $\boldsymbol{x}$ is a positive semidefinite symmetric matrix, i.e., a symmetric matrix whose eigenvalues are positive or 0. Also show that this is the case for the matrix $\boldsymbol{X} = \sum_{\alpha=1}^{N} \boldsymbol{x}_\alpha \boldsymbol{x}_\alpha^\top$ defined by multiple vectors $\boldsymbol{x}_1$, ..., $\boldsymbol{x}_N$, too.

6.3. Show that $\mathrm{tr}(\boldsymbol{x}\boldsymbol{x}^\top) = \|\boldsymbol{x}\|^2$ holds for any vector $\boldsymbol{x}$. Also show that $\mathrm{tr}(\sum_{\alpha=1}^{N} \boldsymbol{x}_\alpha \boldsymbol{x}_\alpha^\top) = \sum_{\alpha=1}^{N} \|\boldsymbol{x}_\alpha\|^2$ holds for any multiple vectors $\boldsymbol{x}_1$, ..., $\boldsymbol{x}_N$.

6.4. Write down explicitly the surface of Eq. (6.10) in three dimensions when $\boldsymbol{\Sigma}$ is a diagonal matrix.

6.5. Show that the ellipsoid given by Eq. (6.10) has its center at the expectation $\bar{\boldsymbol{x}}$ with the eigenvectors $\boldsymbol{u}_i$ of the covariance matrix $\boldsymbol{\Sigma}$ as its axes of symmetry and that the radius in each directions is the standard deviation σ_i of the error in that direction.

6.6. Write $\hat{\boldsymbol{x}}_\alpha = \begin{pmatrix} \hat{x}_{i\alpha} \end{pmatrix}$, and show that the diagonal element S_{ii} of the sample covariance matrix $\boldsymbol{S}$ of Eq. (6.22) is the variance of $\hat{x}_{i\alpha}$ and its non-diagonal element S_{ij}, $i \neq j$ is the sample covariance of $x_{i\alpha}$ and $x_{j\alpha}$.

Chapter 7

Fitting Spaces

7.1 Fitting Subspaces

Given N points $\boldsymbol{x}_1$, ..., $\boldsymbol{x}_N$ in the n-dimensional space $\mathcal{R}^n$, we consider the problem of finding an r-dimensional subspace that is the closest to them, where we assume that $N \geq r$. If $n = 3$ and $r = 1$, for example, this is the problem of line fitting: we want to find a line passing through the origin that is as close to the given N points as possible. For $n = 3$ and $r = 2$, this is plane fitting: we compute a plane passing through the origin that is close o the given N points (Fig. 7.1). Here, the "closeness" is measured by the sum of square distances.

Finding a subspace is equivalent to finding a basis that spans the subpace. Let $\boldsymbol{u}_1$, ..., $\boldsymbol{u}_r$ be an orthonormal basis of the r-dimensional subspace $\mathcal{U}$ to be fitted, and let $\{\boldsymbol{u}_1, ..., \boldsymbol{u}_n\}$ be its extension to an orthonormal basis of the entire $\mathcal{R}^n$. If follows that, put another way, the problem is to find an orthonormal basis $\{\boldsymbol{u}_i\}$ of $\mathcal{R}^n$ such that the subspace $\mathcal{U}$ spanned by its first r vectors $\boldsymbol{u}_1$, ..., $\boldsymbol{u}_r$ is as close to the given N points as possible.

The distance of each point $\boldsymbol{x}_\alpha$ to the subspace $\mathcal{U}$ equals the length of the rejection $\boldsymbol{P}_{\mathcal{U}^\perp}\boldsymbol{x}_\alpha$ from $\mathcal{U}$ からの反 (Fig. 7.2), where $\boldsymbol{P}_{\mathcal{U}} = \sum_{i=r+1}^{n} \boldsymbol{u}_i\boldsymbol{u}_i^\top$ is the projection matrix onto the orthogonal complement $\mathcal{U}^\perp$ of $\mathcal{U}$ ($\hookrightarrow$ Eq. (1.11)). Hence, the sum of square distances of the N points $\boldsymbol{x}_1$, ..., $\boldsymbol{x}_N$ from the subspace $\mathcal{U}$ is given by Eq. (7.1). From Eq. (1.12), this is rewritten as Eq. (7.2). Hence, minimizing the sum of squares of Eq. (7.1) is equivalent to minimizing the sum of square projected lengths onto the subspace $\mathcal{U}$ given by Eq. (7.3).

7.2 Hierarchical Fitting

First, we consider the problem of fitting a one-dimensional subspace. Let $\boldsymbol{v}$ (a unit vector) be its basis. The projected length of each point $\boldsymbol{x}_\alpha$ onto that direction is $\langle \boldsymbol{x}_\alpha, \boldsymbol{v} \rangle$ ($\hookrightarrow$ Eq. (1.16), Fig. 7.3). Hence, the sum of their squares over all points is given by Eq. (7.4), where we define the $n \times n$ matrix $\boldsymbol{\Sigma}$ by Eq. (7.5). This matrix is called by many different names [1], including the "moment matrix" and the "scatter matrix". In the following, we call it the *covariance matrix*, borrowing from statistics, at the risk of possible confusion but for convenience' sake. In statistics terms, this equals the sample covariance matrix of the N sample data $\boldsymbol{x}_\alpha$ around the origin, i.e., by regarding the origin as the mean, multiplied by N ($\hookrightarrow$ Eq. (6.22)).

Equation (7.4) is a quadratic form of a symmetric matrix $\boldsymbol{\Sigma}$ in unit vector $\boldsymbol{v}$. Hence, the vector $\boldsymbol{v}$ that maximizes this is the unit eigenvector of the matrix $\boldsymbol{\Sigma}$ for the maximum eigenvalue, and the resulting value of K equals that maximum eigenvalue of $\boldsymbol{S}$ ($\hookrightarrow$ Appendix A.10). By construction, $\boldsymbol{\Sigma}$ is a positive semidefinite symmetric matrix, and its eigenvalues are all nonnegative ($\hookrightarrow$ Problem 6.2). Let $\sigma_1^2 \geq \cdots \geq \sigma_n^2 \geq 0$ be its eigenvalues. Then, $\boldsymbol{\Sigma}$ has the spectral decomposition of Eq. (7.6) ($\hookrightarrow$ Eq. (2.3)). From this observation, we conclude that the basis of the one-dimensional subspace $\mathcal{U}_1$ that best fits to the point set $\{\boldsymbol{x}_\alpha\}$, $\alpha = 1, ..., N$, is given by $\boldsymbol{v} = \boldsymbol{u}_1$ and that the resulting sum of the square projected lengths equals σ_1^2.

The obtained direction $\boldsymbol{u}_1$ indicates the orientation in which the N points $\{\boldsymbol{x}_\alpha\}$ spread to the largest extent (Fig. 7.4). If the set $\{\boldsymbol{x}_\alpha\}$ approximately spreads linearly, its distribution is well described by a line in the direction of $\boldsymbol{u}_1$. However, if the points spread in other directions, too, this approximation is not sufficient. So, we want to find a direction $\boldsymbol{v}$ that is orthogonal to $\boldsymbol{u}_1$ along which the sum of the square projected lengths is maximized. The square projected length onto the direction of $\boldsymbol{v}$ is again given by Eq. (7.4). The unit vector $\boldsymbol{v}$ that minimizes it subject to the condition $\langle \boldsymbol{v}, \boldsymbol{u}_1 \rangle = 0$ is given by $\boldsymbol{u}_2$ of the spectral decomposition Eq. (7.6) of $\boldsymbol{\Sigma}$, and the corresponding value of K equals σ_2^2 ($\hookrightarrow$ Appendix A.10). The vector $\boldsymbol{u}_2$ indicates the direction in which the spread of the N points $\{\boldsymbol{x}_\alpha\}$ is the second largest.

From this observation, we conclude that the basis of the two-dimensional subspace $\mathcal{U}_2$ that best fits to $\{\boldsymbol{x}_\alpha\}$ is given by $\boldsymbol{u}_1$ and $\boldsymbol{u}_2$. Since $\boldsymbol{u}_1$ and $\boldsymbol{u}_2$ are mutually orthogonal, the sum of the square projected lengths K onto $\mathcal{U}$ is the sum of the corresponding values for $\boldsymbol{u}_1$ and $\boldsymbol{u}_2$, namely $K =$

[1] The terms "moment matrix" and "scatter matrix" are both borrowed from physics.

$\sigma_1^2 + \sigma_2^2$.

By the same argument, we see that the direction in which the spread is the third largest is given by $\boldsymbol{u}_3$ in Eq. (7,6); $\boldsymbol{u}_1$, $\boldsymbol{u}_2$, and $\boldsymbol{u}_3$ span the subspace $\mathcal{U}_3$ that best fits to $\{\boldsymbol{x}_\alpha\}$, and the sum of the projected lengths is $K = \sigma_1^2 + \sigma_2^2 + \sigma_3^2$. Repeating this argment, we see that the basis of the r-dimensional subspace $\mathcal{U}_r$ that best fits to $\{\boldsymbol{x}_\alpha\}$ is $\boldsymbol{u}_1$, ..., $\boldsymbol{u}_r$ and that the sum of the square projected lenghts is $K = \sigma_1^2 + \cdots + \sigma_r^2$.

From Eqs. (7.2) and (7,3), we obtain $J = \sum_{\alpha=1}^N \|\boldsymbol{x}_\alpha\|^2 - K$. From Eq. (7.5), we see that $\mathrm{tr}\boldsymbol{\Sigma} = \sum_{\alpha=1}^N \|\boldsymbol{x}_\alpha\|^2$ ($\hookrightarrow$ Problem 6.3), but since Eq. (7.7) holds from Eq. (7.6) ($\hookrightarrow$ Problem 7.1). Hence, the sum of square distance to $\mathcal{U}_r$ is given by Eq. (7.8), which we call the *residual sum of squares* or the *residual* for short. Since $\sigma_1^2 \geq \cdots \geq \sigma_n^2$, we obtain a smaller residual J as we increase the dimension r of the fitting.

7.3 Fitting by Singular Value Decomposition

The argument of the preceding section shows that an r-dimensional subspace $\mathcal{U}_r$ that best fits to N points $\{\boldsymbol{x}_\alpha\}$, $\alpha = 1$, ..., N, is obtained by first computing the covariance matrix $\mathcal{U}_r$ of Eq. (7.5) and then computing the spectral decomposition of Eq.(7.6).

On the other hand, consider the $n \times N$ matrix $\boldsymbol{X}$ of Eq. (7.9) consisting of vectors $\boldsymbol{x}_\alpha$, $\alpha = 1$, ..., N, as its columns. Then, the covariance matrix $\boldsymbol{\Sigma}$ of Eq. (7.5) is given by Eq. (7.10). Since we are assuming that $N \geq n$, the singular value decomposition of $\boldsymbol{X}$ is given by Eq. (7.11), because the eigenvalues of $\boldsymbol{\Sigma} = \boldsymbol{X}\boldsymbol{X}^\top$ equals the square eigenvalues of $\boldsymbol{X}$ ($\hookrightarrow$ Eq. (3.2)). Moreover, the singular vectors $\boldsymbol{u}_i$ and $\boldsymbol{v}_i$ are, respectively, the eigenvectors of $\boldsymbol{X}\boldsymbol{X}^\top$ and $\boldsymbol{X}^\top\boldsymbol{X}$. It follows that for fitting an r-dimensional subspace $\mathcal{U}_r$ to N points $\{\boldsymbol{x}_\alpha\}$, $\alpha = 1$, ..., N, we may alternatively compute the singular value decomposition of the matrix $\boldsymbol{X}$ of Eq. (7.9) defined by the N points in the form of Eq. (7.11). Then, the left singular vectors $\boldsymbol{u}_1$, ..., $\boldsymbol{u}_r$ provide the basis of $\mathcal{U}_r$, and the residual is given by $J = \sum_{i=r+1}^n \sigma_i^2$.

Thus, the use of the spectral decomposition and the use of the singular value decomposition both give the same result. In actual applications, however, we should use the singular value decomposition. This is for the sake of computational efficiency. Computations involving matrices and vectors consist of computations of "sums of products". Computing the sum of n products requires n multiplications and $n-1$ additions/subtractions. Hence, disregarding the term -1, we can view

the number of multiplications and the number of additions/subtractions as approximately equal. For complexity analysis, therefore, it is sufficient to evaluate the number of multiplications. For spectral decomposition, we first compute the covariance matrix $\mathbf{\Sigma}$ by Eq. (7.10), which requires n^2N multiplication (this is the same if Eq. (7.5) is used). The complexity of the spectral decomposition, i.e. the computation of eigenvalues and eigenvectors, of an $n \times n$ may differ from algorithm to algorithm but is approximately n^3. Hence, the total complexity of computing $\mathbf{\Sigma}$ and its spectral decomposition is approximately $n^2(N+n)$. On the other hand, the complexity of the singular value decomposition of an $n \times N$ matrix is approximately n^2N for $n \leq N$ and approximately nN^2 for $N \leq n$. Hence, the singular value decomposition runs overwhelmingly efficient when $N \ll n$. Even if for $n \leq N$, we can save nearly equivalent time for eigenvalue and eigenvector computation of the covariance matrix.

This time saving is often underestimated. Pattern information processing involves a large amount of data, and usually iterations are required for accuracy improvement. It is not uncommon, for instance, that the number of point data extracted from multiple images is as large as hundreds of thousands. In such a case, several hours of computation can sometimes be reduced to several seconds by simply replacing spectral decomposition computation by singular value computation.

7.4 Fitting Affine Spaces

Subspace fitting is a generalization of fitting to a point sequence a line passing through the origin and a plane passing through the origin. In practice, however, we often need to fit a line that does not pass through the origin and a plane that does not pass through the origin. This type of fitting is generalized to "afine space fitting". An *affine space* is a translation of a subspace. An r-dimensional affine space $\mathcal{A}_r$ is specified by a point $\boldsymbol{g}$ in the n-dimensional space $\mathcal{R}^n$ and r linearly independent vectors $\boldsymbol{u}_1$, ..., $\boldsymbol{u}_r$ starting from it, and is the set of all points that are written as Eq. (7.12) for arbitrary c_1, ..., c_r (Fig. 7.5). Without losing generality, we can let the basis $\{\boldsymbol{u}_i\}$, $i = 1, ..., r$, be an orthonormal system. Alternatively, we can define an r-dimensional affine space by specifying $r + 1$ points in the n-dimensional space $\mathcal{R}^n$ through which it passes, in such a way that whichever point of it is regarded as the origin O, the remaining r points span an r-dimensional subspace. Such $r + 1$ points are said be *in general position* ($\hookrightarrow$ Problem 7.2).

Given N points $\{\boldsymbol{x}_\alpha\}$, $\alpha = 1, ..., N$, in $\mathcal{R}^n$, we consider the problem of finding an r-dimensional

afine space $\mathcal{A}_r$ that approximates them, where we assume that $N \geq r+1$. The affine space $\mathcal{A}_r$ is specified by a point $\boldsymbol{g}$ it passes through and an orthonormal basis $\{\boldsymbol{u}_i\}$ starting from it.

First, we need to specify the point $\boldsymbol{g}$. This can be regarded as a problem of fitting an 0-dimensional affine space (= one point) to the N points $\{\boldsymbol{x}_\alpha\}$. So, we choose $\boldsymbol{g}$ to be a point that minimizes the sum of square distances $\sum_{\alpha=1}^{N} \|\boldsymbol{x}_\alpha - \boldsymbol{g}\|^2$. Such a point is given by the centroid of the N points $\{\boldsymbol{x}_\alpha\}$ given by Eq. (7.13) ($\hookrightarrow$ Problem 7.3).

If $\boldsymbol{g}$ is determined, all we need to do is, according to the argument in the preceding sections, fit an r-dimensional subspace to vectors $\{\boldsymbol{x}_\alpha - \boldsymbol{g}\}$, regarding g as the origin. Namely, we compute the covariance matrix $\boldsymbol{\Sigma}$ of Eq. (7.14) around $\boldsymbol{g}$ ($\hookrightarrow$ Problem 7.4). If its spectral decomposition is written in the form of Eq. (7.6), the eigenvectors $\boldsymbol{u}_1$, ..., $\boldsymbol{u}_r$ span the affine space $\mathcal{A}_r$ around $\boldsymbol{g}$. The residual, i.e., the sum of square distances of individual points $\boldsymbol{x}_\alpha$ to $\mathcal{A}_r$, is given by $K = \sigma_{r+1}^2 + \cdots + \sigma_n^2$.

However, as pointed out in the preceding section, it is more efficient to compute the singular value decomposition of the matrix of Eq. (7.15) consisting of data points, *without computing the covariance matrix*, and then obtaining the basis vectors $\boldsymbol{u}_1$, ..., $\boldsymbol{u}_r$.

Example. Line fitting in the plane

We want to fit a line to N points (x_1, y_1), ..., (x_N, y_N) given in the plane, First, we compute the centroid $(g_x, g_y) = \sum_{\alpha=1}^{N}(x_\alpha, y_\alpha)/N$ and difine the matrix $\boldsymbol{X}$ of Eq. (7.16). Its singular value decomposition has the form of Eq. (7.17). This indicates that the line to be fitted passes through (g_x, g_y) and extends in the direction of $(u_{11}, u_{21})^\top$ (Fig. 7.6). The equation of the fitted line is given by Eq. (7.18).

Example. Plane fitting in the space

We want to fit a plane to N points (x_1, y_1, z_1), ..., (x_N, y_N, z_N) given in the space. First, we compute the centroid $(g_x, g_y, g_z) = \sum_{\alpha=1}^{N}(x_\alpha, y_\alpha, z_\alpha)/N$ and define the matrix $\boldsymbol{X}$ of Eq. (7.19). Its singular decomposition has the form of Eq. (7.20). This indicates that the plane to be fitted passes through (g_x, g_y, g_z) and extends in the directions of $(u_{11}, u_{21}, u_{31})^\top$ and $(u_{12}, u_{22}, u_{32})^\top$ (Fig. 7.7). The vector $(u_{13}, u_{23}, u_{33})^\top$, which is orthogonal to both of them, is the unit surface normal, and the equation of the plane is given by Eq. (7.21).

The technique of computing the spectral decomposition of the covariance matrix of Eq. (7.14)

and hierarchically fitting r-dimensional affine spaces $\mathcal{A}_r$, which is mathematically equivalent to subpace fitting, is used in various problems of engineering and is called by many different names. For signal and pattern recognition applications, it is called the *Karhunen-Loéve expansion*, or the *KL-expansion* for short.. By this, we can represent signals and patterns with respect to as small a number of basis vectors as possible as long as the residual J can be tolerable and make the transmission and display of the data efficient. This is called data compression or image compression.

In statistics, it is called the *principal component analysis*: we can grasp the characteristics of multidimensional statistical data, extract a small number of statistics that can describe them well, and do predictions and tests. In computer vision applications, we describe the camera images and the three-dimensional structures reconstructed from them in terms of lines and planes optimally fitted to them. We can also reduce many video analysis problems to fitting of subspaces and affine spaces in a high-dimensional data space.

Problems of Chapter 7

7.1. Let λ_1, ..., λ_n be the eigenvalues of an $n \times n$ symmetric matrix $\boldsymbol{A}$. Show that Eq. (7.22) holds.

7.2. Show that the condition for $n+1$ points $\boldsymbol{x}_0$, $\boldsymbol{x}_1$, ..., $\boldsymbol{x}_n$ in $\mathcal{R}^n$ to be in general position is given by Eq. (7.23), where the left side is the determinant of an $(n+1) \times (n+1)$ matrix.

7.3. Show that the point $\boldsymbol{g}$ that minimizes the square sum $\sum_{\alpha=1}^{N} \|\boldsymbol{x}_\alpha - \boldsymbol{g}\|^2$ for N points $\{\boldsymbol{x}_\alpha\}$, $\alpha = 1, ..., N$, is given by the centroind $\boldsymbol{g}$ given by Eq. (7.13).

7.4. Show that the covariance matrix $\boldsymbol{\Sigma}$ of Eq. (7.14) is also written in the form of Eq. (7.24).

Chapter 8

Matrix Factorization

8.1 Matrix Factorization

Suppose we want to express an $m \times n$ matrix $\boldsymbol{A}$ as the product of two matrices $\boldsymbol{A}_1$ and $\boldsymbol{A}_2$ in the form of Eq. (8.1), where $\boldsymbol{A}_1$ and $\boldsymbol{A}_2$ are $m \times r$ and $r \times n$ matrices, respectively. We assume $r \leq m$, n. We call this problem matrix *factorization*. When such a problem appears in engineering applications, usually some properties that $\boldsymbol{A}_1$ and $\boldsymbol{A}_2$ are required to satisfy are imposed.

The decomposition of the form of Eq. (8.1) is not unique. In fact, if such matrices $\boldsymbol{A}_1$ and $\boldsymbol{A}_2$ are obtained, the matrices in the form of Eq. (8.2) for an arbitrary $r \times r$ nonsingular matrix $\boldsymbol{C}$ satisfies $\boldsymbol{A}_1\boldsymbol{A}_2 = \boldsymbol{A}_1'\boldsymbol{A}_2'$. In a real application, we first tentatively compute some matrices $\boldsymbol{A}_1$ and $\boldsymbol{A}_2$ that satisfy Eq. (8.1) and then find the nonsingular matrix $\boldsymbol{C}$ in such a way that the required properties imposed on the matrices $\boldsymbol{A}_1'$ and $\boldsymbol{A}_2'$ of Eq. (8.2) are satisfied.

If no special dependencies exist among columns and rows of a matrix, its rank generally coincides with the smaller of the numbers of columns and rows. Assume that matrices $\boldsymbol{A}_1'$ and $\boldsymbol{A}_2'$ both have rank r. It is known that the rank of the product of two matrices does not exceed the rank of either one. Namely, Eq. (8.3) holds for any matrices $\boldsymbol{A}$ and $\boldsymbol{B}$ for which their product can be defined.

This is shown as follows. Let $\boldsymbol{A}$ and $\boldsymbol{B}$ be $l \times m$ and $m \times n$ matrices, respectively. An $l \times m$ matrix $\boldsymbol{A}$ defines a linear mapping from $\mathcal{R}^m$ to $\mathcal{R}^l$. We write $\boldsymbol{A}(\mathcal{R}^m)$ for the image of $\mathcal{R}^m$ by $\boldsymbol{A}$, i.e., the subspace spanned by the vectors obtained by mapping the basis of $\mathcal{R}^m$ by $\boldsymbol{A}$. The dimension of $\boldsymbol{A}(\mathcal{R}^m)$ (= the number of independent columns of $\boldsymbol{A}$) is rank($\boldsymbol{A}$). Similarly, an $m \times n$ matrix $\boldsymbol{B}$ defines a linear mapping from $\mathcal{R}^n$ to $\mathcal{R}^m$, and the dimension of $\boldsymbol{B}(\mathcal{R}^n)$ is rank($\boldsymbol{B}$). On the other hand, since $(\boldsymbol{AB})(\mathcal{R}^n)$ is obtained by first mapping $\mathcal{R}^n$ by $\boldsymbol{B}$ and then mapping it by $\boldsymbol{A}$, it is a subset of $\boldsymbol{A}(\mathcal{R}^m)$. Hence, the dimension of $(\boldsymbol{AB})(\mathcal{R}^n)$ (= rank($\boldsymbol{AB}$)) does not exceed

the dimension of $\boldsymbol{A}(\mathcal{R}^m)$ (= rank($\boldsymbol{A}$)). Thus, we obtain rank($\boldsymbol{AB}$) $\leq$ rank($\boldsymbol{A}$). Using the same argument, we obtain rank($\boldsymbol{B}^\top\boldsymbol{A}^\top$) $\leq$ rank($\boldsymbol{B}^\top$). However, the number of linearly independent columns of a matrix equals the number of its linearly independent rows. Hence, rank($\boldsymbol{B}^\top$) = rank($\boldsymbol{B}$) and rank($\boldsymbol{B}^\top\boldsymbol{A}^\top$) = rank($\boldsymbol{AB}$). Consequently, we also obtain rank($\boldsymbol{AB}$) $\leq$ rank($\boldsymbol{B}$).

From this observation, we find that for computing the factorization of Eq. (8.1), the $m \times n$ matrix $\boldsymbol{A}$ must have rank r or less. However, if $\boldsymbol{A}$ involves measurement data, its rank is generally equal to either m or n (the smaller one). Hence, if $r < m, n$, the decomposition of Eq. (8.1) is not possible. In such a case, we compute such $\boldsymbol{A}_1$ and $\boldsymbol{A}_2$ that the decomposition of Eq. (8.1) approximately holds ($\hookrightarrow$ Problem 8.1). This is done by minimally modify $\boldsymbol{A}$ so that it has rank r. To be specific, we constrain the rank as discussed in Sec. 4.4 and replace $\boldsymbol{A}$ by $(\boldsymbol{A})_r$ ($\hookrightarrow$ Footnote 3 of Chapter 4).

Then, we can determine $\boldsymbol{A}_1$ and $\boldsymbol{A}_2$ that satisfy $(\boldsymbol{A})_r = \boldsymbol{A}_1\boldsymbol{A}_2$. This decomposition is not unique. A simple way to obtain a candidate solution is to first compute the singular value decomposition of $(\boldsymbol{A})_r$ in the form of Eq.(8.4), as in Eq. (3.10), and then decompose the diagonal matrix $\boldsymbol{\Sigma}$ in the form $\boldsymbol{\Sigma} = \boldsymbol{\Sigma}_1\boldsymbol{\Sigma}_2$. Finally, we obtain $\boldsymbol{A}_1$ and $\boldsymbol{A}_2$ in the form of Eq. (8.5) Typical decompositions of $\boldsymbol{\Sigma}$ are given by (i), (ii), and (iii) of Eq. (8.6). The diagonal matrix $\boldsymbol{\Sigma}_1 = \boldsymbol{\Sigma}_2$ in (ii) is also written as $\sqrt{\boldsymbol{\Sigma}}$. From this, we also see that the condition for an $m \times n$ matrix $\boldsymbol{A}$ to have rank r or less ($r \leq m, n$) is that it can be written as $\boldsymbol{A} = \boldsymbol{A}_1\boldsymbol{A}_2$ for some $m \times r$ matrix $\boldsymbol{A}_1$ and some $r \times n$ matrix $\boldsymbol{A}_2$.

8.2 Factorization for Motion Image Analysis

Suppose we take images of N points $(X_\alpha, Y_\alpha, Z_\alpha)$, α = 1, ..., N, in the three-dimensional space, using M cameras (or equivalently moving one camera). Suppose the αth point is projected to $(x_{\alpha\kappa}, y_{\alpha\kappa})$ in the image plane of the κth camera (Fig. 8.2).

We define an XYZ coordinate system in the scene whose origin O coincides with the centroid of the N points, so that Eq. (8.7) holds. We assume that all the points are seen by all the cameras and define an image coordinate system in each image whose origin $(0, 0)$ coincides with the centroid of the N image positions, so that Eq (8.8) holds. Then, it is known that $(X_\alpha, Y_\alpha, Z_\alpha)$ and $(x_{\alpha\kappa}, y_{\alpha\kappa})$ approximately satisfy the relationship of Eq. (8.9), where $\boldsymbol{\Pi}_\kappa$ is a 2×3 matrix, called the *camera matrix*, determined by the position and orientation of the κth camera and its internal parameters.

Strictly speaking, the camera imaging geometry is described by a nonlinear relationship, called *perspective projection*. If we ignore the perspective effect, which causes objects in the distance to look small, we obtain the linear approximation of Eq. (8.9). It is known that this approximation holds well when the objects we are viewing are relatively in the distance, e.g., persons standing several meters away, and zoomed in within a relatively small region of the image. Hypothetical cameras for which Eq. (8.9) hold are said to be *affine*.

Arrange all observed points $(x_{\alpha\kappa}, y_{\alpha\kappa})$ $\kappa = 1, ..., M$, $\alpha = 1, ..., N$, in all images in an $2M \times N$ matrix in the form of Eq. (8.10), which we call the *observation matrix*. Arrange all camera matrices $\boldsymbol{\Pi}_\kappa$, $\kappa = 1, ..., M$, and all three-dimensional coordinates $(X_\alpha, Y_\alpha, Z_\alpha)$, $\alpha = 1, ..., N$, in the matrix form of Eq. (8.11). We call the $2M \times 3$ matrix $\boldsymbol{M}$ the *motion matrix* and the $3 \times N$ matrix $\boldsymbol{N}$ the *shape matrix*.

From the definition of the matrix $\boldsymbol{W}$ of Eq. (8.10) and the definition of the matrices $\boldsymbol{M}$ and $\boldsymbol{N}$ of Eq. (8.11), the relationship of Eq. (8.12) holds ($\hookrightarrow$ Problem 8.2). It follows that if the matrix $\boldsymbol{W}$ obtained from the coordinates of the points observed in images is decomposed into the product of the matrices $\boldsymbol{M}$ and $\boldsymbol{S}$ by the method described in the preceding section, all the camera matrices and all the three-dimensional point positions are obtained. This technique of reconstructing the three-dimensional shape from images is called the *factorization method*.

However, the solution is not unique, as pointed out in the preceding section. If $\bar{\boldsymbol{M}}$ and $\bar{\boldsymbol{S}}$ are the true motion matrix and the shape matrix, respectively, the matrices $\bar{\boldsymbol{M}}$ and $\bar{\boldsymbol{S}}$ obtained by the factorization method are related to $\bar{\boldsymbol{M}}$ and $\bar{\boldsymbol{S}}$ by Eq. (8.13) for some 3×3 nonsingular matrix $\boldsymbol{C}$. The second equation of Eq. (8.13) states that each column $(X_\alpha, Y_\alpha, Z_\alpha)^\top$ of $\boldsymbol{S}$ equals multiplication of each column $(\bar{X}_\alpha, \bar{Y}_\alpha, \bar{Z}_\alpha)^\top$ of $\bar{\boldsymbol{S}}$ by some nonsingular matrix $\boldsymbol{C}$. It follows that the computed three-dimensional shape is a linear transformation of the true shape. Since the absolute position is indeterminate[1], it is an *affine transformation* of the true shape.

Affine transformations preserve collinearity and coplanarity (Fig. 8.3), i.e., collinear points are mapped to collinear points, and coplanar points are mapped to coplanar points. As a result, parallel lines and planes are mapped to parallel lines planes. However, scales and angles may change. For example, a cube is mapped to a parallelepiped. Three-dimensional reconstruction up to indeterminacy of affine transformations is called an *affine reconstruction*.

[1]The origin of the coordinate system in the scene is defined by Eq. (8.7) for the sake of computational convenience, the absolute position in the scene is indeterminate.

In order to remove this indeterminacy to obtain a shape with correct angles, which we call a *Euclidean reconstruction*[2], we need to specify the indeterminate matrix $\boldsymbol{C}$, using some knowledge or constraint, which we call the *metric condition*. One possibility is the use of the knowledge about the three-dimensional scene. For example, we require a particular edge to be orthogonal to a particular edge and determine the matrix $\boldsymbol{C}$ so that the second equation of Eq. (8.13) is satisfied. Another possibility is the use of the knowledge about the camera. For this, we model the camera imaging geometry in a parametric form and express each $\boldsymbol{\Pi}_\kappa$ in terms of unknown parameters. Then, we determine the matrix $\boldsymbol{C}$ so that the first equation of Eq. (8.13) is satisfied. To be specific, the first equation of Eq. (8.13) leads to multiple equalities, from which we can determine the unknown paramers of each camera matrix $\boldsymbol{\Pi}_\kappa$ and the unknown matrix $\boldsymbol{C}$. To this end, various parametric affine camera models are proposed[3].

Problems of Chapter 8

8.1. Show that an $m \times n$ matrix $\boldsymbol{A}$ has rank r or less ($r \leq m, n$) if and only if it is written as $\boldsymbol{A} = \boldsymbol{A}_1 \boldsymbol{A}_2$ for some $m \times r$ matrix $\boldsymbol{A}_1$ and some $r \times n$ matrix $\boldsymbol{A}_2$.

8.2. (1) The αth column of Eq. (8.10) lists the x- and y-coordinates of the αth point over the M images, which can be seen as the "trajectory" of the αth point. Namely, the trajectory of each point is a point in a $2M$-dimensional space. Show that Eq. (8.12) implies that the N points that represent the trajectories in the $2M$-dimensional space are all included in a three-dimensional subspace.

(2) Show how to compute an orthonormal basis of that three-dimensional subspace, by taking into consideration that the decomposition of Eq. (8.12) is for hypothetical cameras, i.e., affine cameras, and that Eq. (8.12) does not exactly hold for the observation matrix $\boldsymbol{W}$ obtained from real cameras.

[2]Since the absolute scale is indeterminate from images alone (↪ Sec. 6.3), we should call it a "similar" reconstruction to be strict, but this term is widely used.

[3]Typical affine camera models include "orthographic projection", "weak perspective projection", and "paraperspective projection".

Appendix A

Fundamentals of Linear Algebra

A.1 Linear Mappings and Matrices

A mapping $f(\,\cdot\,)$ from the n-dimensional space $\mathcal{R}^n$ to the m-dimensional space $\mathcal{R}^m$ is a *linear mapping* if Eq. (A.1) holds for arbitrary $\boldsymbol{u}$, $\boldsymbol{v} \in \mathcal{R}^n$ and an arbitrary real number c, i.e., if *a sum corresponds to a sum and a constant multiple corresponds to a constant multiple*.

Suppose a linear mapping $f(\,\cdot\,)$ maps a vector $\boldsymbol{u} \in \mathcal{R}^n$ to a vector $\boldsymbol{u}' \in \mathcal{R}^m$. If $\boldsymbol{u}$ is a column vector whose ith component is u_i, which we abbreviate to $\boldsymbol{u} = \Big(u_i\Big)$, we can write it as Eq. (A.2), where $\boldsymbol{e}_j$ is the n-dimensional vector whose jth component is 1 and whose other components are all 0. We call the set $\{\boldsymbol{e}_1, ..., \boldsymbol{e}_n\}$ the *natural basis* of $\mathcal{R}^n$. Similarly, we can write the vector $\boldsymbol{u}' = \Big(u'_i\Big) \in \mathcal{R}^m$ in the form of Eq. (A.3), using the natural basis $\{\boldsymbol{e}'_1, ..., \boldsymbol{e}'_m\}$ of $\mathcal{R}^m$.

The mapping of $\boldsymbol{u} \in \mathcal{R}^n$ to $\boldsymbol{u}' \in \mathcal{R}^m$ by $f(\,\cdot\,)$ is given by Eq. (A.4). Since $f(\boldsymbol{e}_j)$ is a vector of $\mathcal{R}^m$, it is expressed as a linear combination of the natural basis $\{\boldsymbol{e}'_1, ..., \boldsymbol{e}'_m\}$ of $\mathcal{R}^m$ in the form of Eq. (A.5). Using this, we obtain Eq. (A.6). Comparing this with Eq. (A.3), we see that Eq. (A.7) holds. This means that the vector $\boldsymbol{u}' = \Big(u'_i\Big)$ is obtained by multiplying the vector $\boldsymbol{u} = \Big(u_i\Big)$ by a matrix whose (i, j) element is a_{ij}, which we abbreviate to $\Big(a_{ij}\Big)$, i.e., Eq. (A.8) holds. Thus, we conclude that *a linear mapping from $\mathcal{R}^n$ to $\mathcal{R}^m$ is represented by multiplication of an $m \times n$ matrix* $\boldsymbol{A} = \Big(a_{ij}\Big)$.

A.2 Inner Product and Norm

The *inner product* $\langle \boldsymbol{a}, \boldsymbol{b} \rangle$ of vectors $\boldsymbol{a} = \Big(a_i\Big)$ and $\boldsymbol{b} = \Big(b_i\Big)$ is defined by Eq. (A.9). It has the properties of (i), (ii), and (iii), i.e., *symmetry*, *linearity*, and *positivity*, respectively.

The norm $\|\boldsymbol{a}\|$ of vector $\boldsymbol{a} = \Big(a_i\Big)$ is defined by Eq. (A.10). A vector with unit norm is said to

be a *unit vector*. The norm has the properties of (i), (ii), and (iii), i.e. (i) *positivity* with equality holding only for $\boldsymbol{a} = \boldsymbol{0}$, (ii) the *Schwarz inequality*, and (iii) the *triangle inequality*, respectively.

Vector $\boldsymbol{a}$ and $\boldsymbol{b}$ are said to be *orthogonal* if $\langle \boldsymbol{a}, \boldsymbol{b} \rangle = 0$. The triangle inequality is obtained by applying the Schwartz inequality (see [7] for the derivation) to Eq. (A.11) and noting that Eq. (A.11) is larger than or equal to $\|\boldsymbol{a}\|^2 - 2\|\boldsymbol{a}\| \cdot \|\boldsymbol{b}\| + \|\boldsymbol{b}\|^2 = (\|\boldsymbol{a}\| - \|\boldsymbol{b}\|)^2$ and smaller than or equal to $\|\boldsymbol{a}\|^2 + 2\|\boldsymbol{a}\| \cdot \|\boldsymbol{b}\| + \|\boldsymbol{b}\|^2 = (\|\boldsymbol{a}\| + \|\boldsymbol{b}\|)^2$. From this, we also see that if $\langle \boldsymbol{a}, \boldsymbol{b} \rangle = 0$, i.e., if $\boldsymbol{a}$ and $\boldsymbol{b}$ are orthogonal, the *Pythagorean theorem* of Eq. (A.12) is obtained.

A.3 Linear Forms

For a constant vector $\boldsymbol{a} = \Big(a_i\Big)$ and a variable vector $\boldsymbol{x} = \Big(x_i\Big)$, Eq. (A.13) is called a *linear form* in $\boldsymbol{x}$. Differentiating this with respect to x_i, we obtain Eq. (A.14). In vector form, it is written as Eq. (A.15), where we define the vector $\nabla_{\boldsymbol{x}}(\cdots)$ by Eq. (A.16). We call this the *gradient* of $\cdots$ and call the symbol ∇ *nabla*.

A.4 Quadratic Forms

For a constant symmetric matrix $\boldsymbol{A} = \Big(a_{ij}\Big)$ and a variable vector $\boldsymbol{x} = \Big(x_i\Big)$, we call Eq. (A.17) a *quadratic form* in $\boldsymbol{x}$. The reason for restricting $\boldsymbol{A}$ to be a symmetric matrix is as follows. A general square matrix $\boldsymbol{A}$is decomposed into the sum of its *symmetric part* $\boldsymbol{A}^{(s)}$ and *anti-symmetric part* $\boldsymbol{A}^{(a)}$ as shown in Eq. (A.18). By definition, $\boldsymbol{A}^{(s)}$ and $\boldsymbol{A}^{(a)}$ are, respectively, a symmetric matrix and an anti-symmetric matrix. If the matrix $\boldsymbol{A}$ in Eq. (A.17) is not symmetric, we substitute Eq. (A.18) and obtain Eq. (A.20). Hence, only the symmetric part of $\boldsymbol{A}$ has a meaning. The reason for $\langle \boldsymbol{x}, \boldsymbol{A}^{(a)}\boldsymbol{x} \rangle = \sum_{i,j=1}^{n} a_{ij}^{(a)} x_i x_j$ being 0 is that for each pair (i, j) the term $a_{ij}^{(a)} x_i x_j$ and the term $a_{ji}^{(a)} x_j x_i$ $(= -a_{ij}^{(a)} x_i x_j)$ cancel each other. Note that $a_{ii}^{(a)} = 0$ for an anti-symmetric matrix by definition.

This observation implies that for an arbitrary $\boldsymbol{x}$, the equality $\langle \boldsymbol{x}, \boldsymbol{A}\boldsymbol{x} \rangle = 0$ does not mean $\boldsymbol{A} = \boldsymbol{O}$. It only means that $\boldsymbol{A}^{(s)}$ (Eq. (A.21)). Similarly, the equality $\langle \boldsymbol{x}, \boldsymbol{A}\boldsymbol{x} \rangle = \langle \boldsymbol{x}, \boldsymbol{B}\boldsymbol{x} \rangle$ for an arbitrary $\boldsymbol{x}$ does not mean $\boldsymbol{A} = \boldsymbol{B}$. It only means that $\boldsymbol{A}^{(s)} = \boldsymbol{B}^{(s)}$ (Eq. (A.22)).

From this consideration, we assume that the matrix $\boldsymbol{A}$ of a quadratic form is symmetric from the beginning. If $\boldsymbol{A}$ is symmetric, then $a_{ij} = a_{ji}$, and hence the terms of Eq. (A.17) that include x_1 are those in Eq. (A.23). Differentiating this with respect to x_1, we obtain $2a_{11}x_1 + 2(a_{12}x_2 + a_{13}x_3 +$

$\cdots + a_{1n}x_n) = 2\sum_{j=1}^{n} a_{1j}x_j$. Since similar results hold for x_2, ..., x_n, too, we obtain Eq. (A.24). Using ∇, we rewrite this in vector form as Eq. (A.25). We see that Eqs. (A.15) and (A.25) are, respectively, extensions of the formulas $d(ax)/dx = a$ and $d(Ax^2)/dx = 2Ax$ for one variable to n variables.

A.5 Bilinear Forms

For a constant matrix $\boldsymbol{A} = \left(a_{ij}\right)$ and variable vectors $\boldsymbol{x} = \left(x_i\right)$ and $\boldsymbol{y} = \left(y_i\right)$, we call Eq. (A.26) a *bilinear form* in $\boldsymbol{x}$ and $\boldsymbol{y}$, for which we observe the fundamental equality of Eq. (A.27). In fact, both sides are equal to $\sum_{i,j=1}^{N} a_{ij}x_iy_j$ from the rule of the product of a matrix and a vector. In contrast to the case of quadratic forms, we see that if $\langle \boldsymbol{x}, \boldsymbol{Ay} \rangle = 0$ for any $\boldsymbol{x}$ and $\boldsymbol{y}$, then $\boldsymbol{A} = \boldsymbol{O}$ (Eq. (A.28)) and that if $\langle \boldsymbol{x}, \boldsymbol{Ay} \rangle = \langle \boldsymbol{x}, \boldsymbol{By} \rangle$ for any $\boldsymbol{x}$ and $\boldsymbol{y}$, then $\boldsymbol{A} = \boldsymbol{B}$ (Eq. (A.29)). From Eqs. (A.15) and (A.27), the identities of Eq.(A.30) are obtained.

A.6 Basis and Expansion

A set of vectors $\boldsymbol{u}_1$, ..., $\boldsymbol{u}_r$ is said to be an *orthonormal system* if they are all unit vectors and orthogonal to each other, i.e., if Eq. (A.31) holds, where δ_{ij} is the *Kronecker delta* (the symbol that take 1 for $i = j$ and 0 for $i \neq j$)..

If an arbitrary vector $\boldsymbol{x}$ can be uniquely expressed as a linear combination of some n vectors $\boldsymbol{u}_1$, ..., $\boldsymbol{u}_n$, they are called the *basis* of that space and n is called the *dimension* of that space. An orthonormal system of n vectors $\{\boldsymbol{u}_1, ..., \boldsymbol{u}_n\}$ constitute a basis of the n-dimensional space $\mathcal{R}^n$, called an *orthonormal basis*.

Expressing a given vector $\boldsymbol{x}$ as a linear combination of an orthonormal basis $\{\boldsymbol{u}_i\}$, $i = 1, ..., n$, in the form of Eq. (A.32) is called *expansion* of x in terms of $\{\boldsymbol{u}_i\}$. The square norm of Eq. (A.32) is written as Eq. (A.33), where we write $\langle \sum_{i=1}^{n} c_i\boldsymbol{u}_i, \sum_{j=1}^{n} c_j\boldsymbol{u}_j \rangle$ instead of $\langle \sum_{i=1}^{n} c_i\boldsymbol{u}_i, \sum_{i=1}^{n} c_i\boldsymbol{u}_i \rangle$ for avoiding the confusion of running indices in the summation. Note that if the Kronecker delta δ_{ij} appears in a summation $\sum$ with respect to i or j or both, only terms for which $i = j$ survive.

Computing the inner product of $\boldsymbol{u}_i$ and Eq. (A.32) and noting that $\{\boldsymbol{u}_i\}$ is an orthonormal system, we obatin Eq. (A.34). Hence, the expansion of Eq. (A.32) is written in the form of Eq. (A.35). Since $\{\boldsymbol{u}_i\}$ is a basis, the expansion expression is unique. From Eq. (A.33), its square norm is written as Eq. (A.36).

A.7 Least-squares Approximation

For an orthonormal system $\{\boldsymbol{u}_i\}$, $i = 1, ..., r$, of r ($\leq n$) vectors, vector $\boldsymbol{x}$ is not necessarily expanded in the form of Eq. (A.32). However, we can determine the expansion coefficients c_i, $i = 1, ..., r$, in such a way that Eq. (A.37) is minimized. Expansion using such coefficients is called the *least-squares approximation*. Equation (A.37) is rewritten as Eq. (A.38). Differentiating this with respect to c_k, we obtain Eq. (A.39). Equating this to 0, we obtain $c_k = \langle \boldsymbol{u}_k, \boldsymbol{x} \rangle$. Hence, the least-squares expansion has the form of Eq. (A.40). This correspond to *truncating the expansion of Eq. (A.33) up to the rth term*.

The set $\mathcal{U}$ of all vectors that can be expressed as linear combinations of $\boldsymbol{u}_1, ..., \boldsymbol{u}_r$ is called the *subspace spanned* by $\boldsymbol{u}_1, ..., \boldsymbol{u}_r$. If $\boldsymbol{u}_1, ..., \boldsymbol{u}_r$ are an orthonormal system, they form the basis of the subspace $\mathcal{U}$, and its dimension is r. The right side of Eq. (A.40) equals the projection $\boldsymbol{P}_{\mathcal{U}}\boldsymbol{x}$ of $\boldsymbol{x}$ onto the subspace $\mathcal{U}$ by the projection matrix $\boldsymbol{P}_{\mathcal{U}} = \boldsymbol{u}_1\boldsymbol{u}_1^\top + \cdots + \boldsymbol{u}_r\boldsymbol{u}_r^\top$ ($\hookrightarrow$ Sec. 1.5). Namely, *least-square approximation equals projection onto a subspace*. From this observation, we see that if the vector $\boldsymbol{x}$ is in the subspace $\mathcal{U}$, Eq. (A.40) holds with equality, i.e., Eq. (A.41) holds. The vectors $\{\boldsymbol{u}_i\}$, $i = 1, ..., r$, are now an orthonormal basis of $\mathcal{U}$, and hence this expansion expression is unique. Its square norm is given by Eq. (A.42).

A.8 Lagrange's Method of Indeterminate Multipliers

The maximum and minimum of a function $f(\boldsymbol{x})$ of variable $\boldsymbol{x}$ is computed by solving Eq. (A.43) if there is no constraint on $\boldsymbol{x}$. If $\boldsymbol{x}$ is constrained to satisfy Eq. (A.44), we introduce a *Lagrange muliplier* λ and consider Eq. (A.45). Differentiating this with respect to x and letting the result be 0, we obtain Eq. (A.46). We can determine $\boldsymbol{x}$ and λ by solving this together with Eq. (A.44). This is called *Lagrange's method of indeterminate multipliers* (see [8] for the derivation).

We should note that what we obtain by this method is in general extreme values. Hence, we need some criteria to judge if the solution is a maximum, a minimum, or other types of extremum including an inflection points. However, if it is known from the properties of the problem that it has a unique maximum or a unique minimum, this is a very convenient and practical method.

If multiple constraints of the form of Eq. (A.47) exist, we introduce Lagrange multipliers $\lambda_1, ..., \lambda_m$ corresponding to individual constraints and consider Eq. (A.48) for computing the maximum or minimum (an extremum in general) of $f(\boldsymbol{x})$, where we write the m Lagrange multipliers and m

constraints of Eq. (A.47) in the vector form of Eq. (A.49). Differentiating Eq. (A.47) with respect to $\boldsymbol{x}$ and letting it be $\mathbf{0}$, we obtain Eq. (A.50). Solving this together with Eq. (A.47), we can determine $\boldsymbol{x}$ and λ_1, ..., λ_m.

A.9 Eigenvalues and Eigenvectors

For an $n \times n$ symmetric matrix $\boldsymbol{A}$, we call the value λ that satisfies Eq.(A.51) an *eigenvalue* of $\boldsymbol{A}$. The vector $\boldsymbol{u}$ ($\neq \mathbf{0}$) is called the corresponding *eigenvector*. Equation (A.51) is rewritten in the form of Eq. (A.52). This is a set of linear equations in $\boldsymbol{u}$. As is well known, this has a solution $\boldsymbol{u}$ $\neq \mathbf{0}$ if and only if the determinant of the coefficient matrix is 0, i.e., when Eq. (A.53) holds. This is called the *characteristic equation*, where $|\cdot|$ denote the determinant and $\phi(\lambda)$ is an nth degree polynomial in λ, called the *characteristic polynomial*. Since Eq. (A.53) is an nth degree polynomial equation with real coefficients, it has in general n solutions in the complex number domain. Hence, matrix $\boldsymbol{A}$ has n eigenvalues and n corresponding eigenvectors. However, for a symmetric matrix, *all eigenvalues are real and the corresponding eigenvectors consist of real components*. This can be shown as follows.

Let λ be an eigenvalue (possibly a complex number) of $\boldsymbol{A}$, and λ the corresponding eigenvector (possibly having complex components). Their definition and its complex conjugate on both sides are written as Eq. (A.54). The inner product of the first equation and $\bar{\boldsymbol{u}}$ on both sides and the inner product of the second equation and $\boldsymbol{u}$ on both sides are given by Eq. (A.55). If we write $\boldsymbol{u}$ $= \left(u_i\right)$ ($\neq \mathbf{0}$), we obtain Eq. (A.56), where $|\cdot|$ denotes the absolute value of a complex number. Since $\boldsymbol{A}$ is symmetric, we obtain Eq. (A.57) ($\hookrightarrow$ Eq. (A.27)). Hence, $\lambda = \bar{\lambda}$, and λ is a real number. A set of simultaneous linear equations $\boldsymbol{Au} = \lambda\boldsymbol{u}$ in unknown $\boldsymbol{u}$ for a matrix $\boldsymbol{A}$ of real elements and a real number λ can be solved using arithmetic operations and substitutions, the resulting solution $\boldsymbol{u}$ also has real components.

Furthermore, we can show that *eigenvectors for different eigenvalues are mutually orthogonal* as follows. If we let $\boldsymbol{u}$ and $\boldsymbol{u}'$ be the eigenvectors of $\boldsymbol{A}$ for eigenvalues λ and λ' ($\lambda \neq \lambda'$), respectively, Eq. (A.58) holds. The inner product of the first equation and $\boldsymbol{u}'$ on both sides and the inner product of the second equation with $\boldsymbol{u}$ on both sides are written as Eq. (A.59). Since $\boldsymbol{A}$ is symmetric, Eq. (A.60) holds ($\hookrightarrow$ Eq. (A.27)). Hence, from Eq. (A.59), we obtain Eq. (A.61), which means $(\lambda - \lambda')\langle \boldsymbol{u}', \boldsymbol{u}\rangle = 0$. Since $\lambda \neq \lambda'$, this implies $\langle \boldsymbol{u}', \boldsymbol{u}\rangle = 0$, i.e.e, $\boldsymbol{u}$ and $\boldsymbol{u}'$ are orthogonal to each

other.

If there is multiplicity among the n eigenvalues, the eigenvectors for multiple eigenvalue are not unique. However, their arbitrary linear combination are also eigenvalues for the same eigenvalue. Hence, we can choose them, using, e.g., the Schmidt orthogonalization ($\hookrightarrow$ Sec. 1.5), to be mutually orthogonal vectors (see [7] for the procedure). As can be seen from Eq. (A.51), if $\boldsymbol{u}$ is an eigenvector, its arbitrary constant multiple $c\boldsymbol{u}$ ($c \neq 0$) is also an eigenvector for the same eigenvalue. As a result the eigenvectors $\{\boldsymbol{u}_i\}$, $i = 1, ..., n$, of a symmetric matrix can be chosen to be an orthonormal system of vectors.

A.10 Maximum and Minimum of a Quadratic Form

Consider a quadratic form $\langle \boldsymbol{v}, \boldsymbol{A}\boldsymbol{v} \rangle$ of an $n \times n$ symmetric matrix $\boldsymbol{A}$ in unit vector $\boldsymbol{v}$. Let $\lambda_1 \geq \cdots \geq \lambda_n$ be the n eigenvalues of $\boldsymbol{A}$, and $\{\boldsymbol{u}_i\}$, $i = 1, ..., n$, the corresponding orthonormal sytem of the corresponding eigenvectors. Since an arbitrary unit vector $\boldsymbol{v}$ can be expanded in the form $\boldsymbol{v} = \sum_{i=1}^{n} c_i \boldsymbol{u}_i$, $\sum_{i=1}^{n} c_i^2 = 1$ ($\hookrightarrow$ A.6), we can rewrite the quadratic form as Eq. (A.62). The equality holds when $c_1 = 1$ and $c_2 = \cdots = c_n = 0$, i.e., when $\boldsymbol{v} = \boldsymbol{u}_1$. Similarly, Eq. (A.63) obtained by reversing the inequality of Eq. (A.62) also holds. Thus, we conclude that *the maximum and minimum of a quadratic form* $\langle \boldsymbol{v}, \boldsymbol{A}\boldsymbol{v} \rangle$ *of a symmetric matrix* $\boldsymbol{A}$ *in unit vector* $\boldsymbol{v}$ *equal the maximum eigenvalue* λ_1 *and the minimum eigenvalue* λ_n *of* $\boldsymbol{A}$*, respectively,* $\boldsymbol{v}$ *being equal to the corresponding unit eigenvectors* $\boldsymbol{u}_1$ *and* $\boldsymbol{u}_n$*, respectively.*

Next, consider a unit vector $\boldsymbol{v}$ orthogonal to $\boldsymbol{u}_1$. An arbitrary unit vector $\boldsymbol{v}$ orthogonal to $\boldsymbol{u}_1$ can be expanded in the form $\boldsymbol{v} = \sum_{i=2}^{n} c_i \boldsymbol{u}_i$, $\sum_{i=2}^{n} c_i^2 = 1$ ($\hookrightarrow$ A.6). Hence, the quadratic form $\langle \boldsymbol{v}, \boldsymbol{A}\boldsymbol{v} \rangle$ can be written as Eq. (A.64). The equality holds when $c_2 = 1$ and $c_3 = \cdots = c_n = 0$, i.e., when $\boldsymbol{v} = \boldsymbol{u}_2$. Hence, $\langle \boldsymbol{v}, \boldsymbol{A}\boldsymbol{v} \rangle$ *for a unit vector* $\boldsymbol{v}$ *orthogonal to* $\boldsymbol{u}_1$ *takes its maximum when* $\boldsymbol{v}$ *equals the unit eigenvector* $\boldsymbol{u}_2$ *for the second largest eigenvalue* λ_2*, the maximum value being* λ_2*.*

By the same argument, we conclude that $\langle \boldsymbol{v}, \boldsymbol{A}\boldsymbol{v} \rangle$ *for a unit vector* $\boldsymbol{v}$ *orthogonal to* $\boldsymbol{u}_1$*, ...,* $\boldsymbol{u}_{m-1}$ *takes its maximum when* $\boldsymbol{v}$ *equals the unit eigenvector* $\boldsymbol{u}_m$ *for the* m*th largest eigenvalue* λ_m*, the maximum being* λ_m*.* The same holds for the minimum: $\langle \boldsymbol{v}, \boldsymbol{A}\boldsymbol{v} \rangle$ *for a unit vector* $\boldsymbol{v}$ *orthogonal to* $\boldsymbol{u}_{n-m}$*, ...,* $\boldsymbol{u}_n$ *takes its minimum when* $\boldsymbol{v}$ *equals the unit eigenvector* $\boldsymbol{u}_{n-m+1}$ *for the* m*th smallest eigenvalue* λ_{n-m+1}*, the maximum being* λ_{n-m+}*.*

問題の解答

第1章

1.1. (1) 行列の積の定義より明らかである．

$$\begin{pmatrix} a_1 \\ \vdots \\ a_m \end{pmatrix} \begin{pmatrix} b_1 & \cdots & b_n \end{pmatrix} = \begin{pmatrix} a_1 b_1 & \cdots & a_1 b_n \\ \vdots & \ddots & \vdots \\ a_m b_1 & \cdots & a_m b_n \end{pmatrix}$$

(2) 上記の行列のトレースは $\sum_{i=1}^{n} a_i b_i = \langle \boldsymbol{a}, \boldsymbol{b} \rangle$ である．

1.2. $\mathcal{U}$ の正規直交基底を $\{\boldsymbol{u}_i\}$, $i = 1, ..., r$ とし，$\overrightarrow{OQ} \in \mathcal{U}$ を $\overrightarrow{OQ} = \sum_{i=1}^{r} c_i \boldsymbol{u}_i$ と表すと，

$$\|\overrightarrow{PQ}\|^2 = \|\overrightarrow{OQ} - \overrightarrow{OP}\|^2 = \|\sum_{i=1}^{r} c_i \boldsymbol{u}_i - \overrightarrow{OP}\|^2 = \langle \sum_{i=1}^{r} c_i \boldsymbol{u}_i - \overrightarrow{OP}, \sum_{j=1}^{r} c_j \boldsymbol{u}_j - \overrightarrow{OP} \rangle$$

と書ける．これを c_i で微分すると

$$\frac{\partial \|\overrightarrow{PQ}\|^2}{\partial c_i} = 2\langle \boldsymbol{u}_i, \sum_{j=1}^{r} c_j \boldsymbol{u}_j - \overrightarrow{OP} \rangle = 2\langle \boldsymbol{u}_i, \overrightarrow{PQ} \rangle$$

となる．最短点ではこれが 0 となるから，$\overrightarrow{PQ}$ は $\mathcal{U}$ の基底 $\{\boldsymbol{u}_i\}$, $i = 1, ..., r$ に直交する．ゆえに $\overrightarrow{OQ}$ は $\overrightarrow{OP}$ の射影である．

1.3. 次のように示せる．

$$\boldsymbol{P}_{\mathcal{U}}^{\top} = \Big(\sum_{i=1}^{r} \boldsymbol{u}_i \boldsymbol{u}_i^{\top} \Big)^{\top} = \sum_{i=1}^{r} \boldsymbol{u}_i \boldsymbol{u}_i^{\top} = \boldsymbol{P}_{\mathcal{U}}$$

$$\boldsymbol{P}_{\mathcal{U}}^2 = \Big(\sum_{i=1}^{r} \boldsymbol{u}_i \boldsymbol{u}_i^{\top} \Big) \Big(\sum_{j=1}^{r} \boldsymbol{u}_j \boldsymbol{u}_j^{\top} \Big) = \sum_{i,j=1}^{r} \boldsymbol{u}_i \boldsymbol{u}_i^{\top} \boldsymbol{u}_j \boldsymbol{u}_j^{\top} = \sum_{i,j=1}^{r} \boldsymbol{u}_i \langle \boldsymbol{u}_i, \boldsymbol{u}_j \rangle \boldsymbol{u}_j^{\top}$$
$$= \sum_{i,j=1}^{r} \delta_{ij} \boldsymbol{u}_i \boldsymbol{u}_j^{\top} = \sum_{i=1}^{r} \boldsymbol{u}_i \boldsymbol{u}_i^{\top} = \boldsymbol{P}_{\mathcal{U}}$$

1.4. $n \times n$ 行列 $\boldsymbol{P}$ が対称行列であれば，よく知られているように，n 個の実数の固有値 $\lambda_1, ..., \lambda_n$ を持ち，対応する固有ベクトル $\boldsymbol{u}_1, ..., \boldsymbol{u}_n$ を正規直交系にとることができる．$\boldsymbol{P}\boldsymbol{u}_i = \lambda_i \boldsymbol{u}_i$ の両辺に左から $\boldsymbol{P}$ を掛けると，

$$\boldsymbol{P}^2 \boldsymbol{u}_i = \lambda_i \boldsymbol{P} \boldsymbol{u}_i = \lambda_i^2 \boldsymbol{u}_i$$

である．しかし，$\boldsymbol{P}$ がべき等なら，左辺は $\boldsymbol{P}\boldsymbol{u}_i = \lambda_i \boldsymbol{u}_i$ である．ゆえに，$\lambda_i = \lambda_i^2$，すなわち，$\lambda_i = 0$, 1 である．$\lambda_1 = \cdots = \lambda_r = 1$, $\lambda_{r+1} = \cdots = \lambda_n = 0$ とすると，

$$\boldsymbol{P}\boldsymbol{u}_i = \boldsymbol{u}_i, \quad i = 1, ..., r, \qquad \boldsymbol{P}\boldsymbol{u}_i = \boldsymbol{0}, \quad i = r+1, ..., n$$

である．これは，式 (1.7) より，$\boldsymbol{P}$ が $\boldsymbol{u}_1$, ..., $\boldsymbol{u}_r$ の張る部分空間への射影行列であることを意味する．

第 2 章

2.1. $\boldsymbol{u}_1$, ..., $\boldsymbol{u}_m$, $\boldsymbol{u}_i \neq \boldsymbol{0}$, $i = 1$, ..., m のある線形結合が $\boldsymbol{0}$ であるとする．

$$c_1\boldsymbol{u}_1 + \cdots + c_m\boldsymbol{u}_m = \boldsymbol{0}$$

両辺と $\boldsymbol{u}_k$ との内積をとると，$\{\boldsymbol{u}_i\}$, $i = 1$, ..., m は互いに直交するから，

$$c_k\langle \boldsymbol{u}_k, \boldsymbol{u}_k\rangle = c_k\|\boldsymbol{u}_k\|^2 = 0$$

であり，$c_k = 0$ である．これは $k = 1$, ..., m に対して成り立つから，$\boldsymbol{u}_1$, ..., $\boldsymbol{u}_m$ の線形結合が $\boldsymbol{0}$ となるのは，係数がすべて 0 のときに限る．ゆえに，$\boldsymbol{u}_1$, ..., $\boldsymbol{u}_m$ は線形独立である．

2.2. $\boldsymbol{a}_i$, $\boldsymbol{b}_i$ の第 j 成分をそれぞれ a_{ji}, b_{ji} と書くと，行列 $\boldsymbol{a}_i\boldsymbol{b}_i^\top$ の (k,l) 要素は $a_{ki}b_{li}$ である（↪ 式 (1.22)）．ゆえに，式 (2.19) の左辺の行列の (k,l) 要素は $\sum_{i=1}^n a_{ki}b_{li}$ である．$\boldsymbol{A} = \begin{pmatrix}\boldsymbol{a}_1 & \cdots & \boldsymbol{a}_n\end{pmatrix} = \Big(a_{ij}\Big)$, $\boldsymbol{B} = \begin{pmatrix}\boldsymbol{b}_1 & \cdots & \boldsymbol{b}_n\end{pmatrix} = \Big(b_{ij}\Big)$ であるから，$\sum_{i=1}^n a_{ki}b_{li}$ は $\boldsymbol{A}\boldsymbol{B}^\top$ の (k,l) 要素に等しい．

2.3. 行列 $\boldsymbol{U}$ の定義より，

$$\boldsymbol{U}^\top\boldsymbol{U} = \begin{pmatrix}\boldsymbol{u}_1^\top \\ \vdots \\ \boldsymbol{u}_n^\top\end{pmatrix}\begin{pmatrix}\boldsymbol{u}_1 & \cdots & \boldsymbol{u}_n\end{pmatrix} = \begin{pmatrix}\langle \boldsymbol{u}_1, \boldsymbol{u}_1\rangle & \cdots & \langle \boldsymbol{u}_1, \boldsymbol{u}_n\rangle \\ \vdots & \ddots & \vdots \\ \langle \boldsymbol{u}_n, \boldsymbol{u}_1\rangle & \cdots & \langle \boldsymbol{u}_n, \boldsymbol{u}_n\rangle\end{pmatrix}$$

である．これが $\boldsymbol{I}$ に等しい必要十分条件は $\langle \boldsymbol{u}_i, \boldsymbol{u}_j\rangle = \delta_{ij}$，すなわち，$\boldsymbol{U}$ の列が正規直交系をなすことである．

2.4. 式 (1.11) は，$\boldsymbol{U}^\top$ が $\boldsymbol{U}$ の逆行列であること，すなわち $\boldsymbol{U}^\top = \boldsymbol{U}^{-1}$ を意味している．ゆえに

$$(\boldsymbol{U}^\top)^\top(\boldsymbol{U}^\top) = \boldsymbol{U}\boldsymbol{U}^\top = \boldsymbol{U}\boldsymbol{U}^{-1} = \boldsymbol{I}$$

であり，$\boldsymbol{U}^\top$ も直交行列である．したがって，$\boldsymbol{U}$ の行も正規直交系をなしている．

2.5. 次のように示せる．

$$\begin{aligned}\boldsymbol{A}^{-1}\boldsymbol{A} &= \Big(\sum_{i=1}^n \frac{\boldsymbol{u}_i\boldsymbol{u}_i^\top}{\lambda_i}\Big)\Big(\sum_{j=1}^n \lambda_j\boldsymbol{u}_j\boldsymbol{u}_j^\top\Big) = \sum_{i,j=1}^n \frac{\lambda_j}{\lambda_i}\boldsymbol{u}_i\boldsymbol{u}_i^\top\boldsymbol{u}_j\boldsymbol{u}_j^\top = \sum_{i,j=1}^n \frac{\lambda_j}{\lambda_i}\boldsymbol{u}_i\langle \boldsymbol{u}_i, \boldsymbol{u}_j\rangle\boldsymbol{u}_j^\top \\ &= \sum_{i,j=1}^n \frac{\lambda_j}{\lambda_i}\delta_{ij}\boldsymbol{u}_i\boldsymbol{u}_j^\top = \sum_{i=1}^n \boldsymbol{u}_i\boldsymbol{u}_i^\top = \boldsymbol{I}\end{aligned}$$

2.6. 式 (2.17) から，次のように示せる．

$$\begin{aligned}(\sqrt{\boldsymbol{A}})^2 &= \Big(\sum_{i=1}^n \sqrt{\lambda_i}\boldsymbol{u}_i^\top\Big)\Big(\sum_{j=1}^n \sqrt{\lambda_j}\boldsymbol{u}_j^\top\Big) = \sum_{i,j=1}^n \sqrt{\lambda_i\lambda_j}\boldsymbol{u}_i\boldsymbol{u}_i^\top\boldsymbol{u}_j\boldsymbol{u}_j^\top = \sum_{i,j=1}^n \sqrt{\lambda_i\lambda_j}\boldsymbol{u}_i\langle \boldsymbol{u}_i, \boldsymbol{u}_j\rangle\boldsymbol{u}_j^\top \\ &= \sum_{i,j=1}^n \sqrt{\lambda_i\lambda_j}\delta_{ij}\boldsymbol{u}_i\boldsymbol{u}_j^\top = \sum_{i=1}^n \lambda_i\boldsymbol{u}_i\boldsymbol{u}_i^\top = \boldsymbol{A}\end{aligned}$$

また，式 (2.18) の第 1 式と式 (2.9) からも，次のように示せる．

$$\begin{aligned}(\sqrt{\boldsymbol{A}})^2 &= \boldsymbol{U}\begin{pmatrix}\sqrt{\lambda_1} & & \\ & \ddots & \\ & & \sqrt{\lambda_n}\end{pmatrix}\boldsymbol{U}^\top\boldsymbol{U}\begin{pmatrix}\sqrt{\lambda_1} & & \\ & \ddots & \\ & & \sqrt{\lambda_n}\end{pmatrix}\boldsymbol{U}^\top \\ &= \boldsymbol{U}\begin{pmatrix}\sqrt{\lambda_1} & & \\ & \ddots & \\ & & \sqrt{\lambda_n}\end{pmatrix}\begin{pmatrix}\sqrt{\lambda_1} & & \\ & \ddots & \\ & & \sqrt{\lambda_n}\end{pmatrix}\boldsymbol{U}^\top \\ &= \boldsymbol{U}\begin{pmatrix}\lambda_1 & & \\ & \ddots & \\ & & \lambda_n\end{pmatrix}\boldsymbol{U}^\top = \boldsymbol{A}\end{aligned}$$

2.7. 次式が成り立つ．

$$(\boldsymbol{A}^{-1})^N\boldsymbol{A}^N = \boldsymbol{A}^{-1}\cdots\boldsymbol{A}^{-1}\boldsymbol{A}\cdots\boldsymbol{A} = \boldsymbol{I}$$

これは $(\boldsymbol{A}^{-1})^N$ が $\boldsymbol{A}^N$ の逆行列であること，すなわち $(\boldsymbol{A}^{-1})^N = (\boldsymbol{A}^N)^{-1}$ を示している．

第 3 章

3.1. 明らかに $\boldsymbol{A}\boldsymbol{A}^\top$ も $\boldsymbol{A}^\top\boldsymbol{A}$ も対称行列である．$\boldsymbol{A}\boldsymbol{A}^\top$ が固有値 λ，固有ベクトル $\boldsymbol{u}$ $(\neq \boldsymbol{0})$ を持つとして，$\boldsymbol{A}\boldsymbol{A}^\top\boldsymbol{u} = \lambda\boldsymbol{u}$ の両辺と $\boldsymbol{u}$ の内積をとると，

$$\langle\boldsymbol{u}, \boldsymbol{A}\boldsymbol{A}^\top\boldsymbol{u}\rangle = \lambda\langle\boldsymbol{u}, \boldsymbol{u}\rangle = \lambda\|\boldsymbol{u}\|^2$$

であるが,

$$\langle\boldsymbol{u}, \boldsymbol{A}\boldsymbol{A}^\top\boldsymbol{u}\rangle = \langle\boldsymbol{A}^\top\boldsymbol{u}, \boldsymbol{A}^\top\boldsymbol{u}\rangle = \|\boldsymbol{A}^\top\boldsymbol{u}\|^2 \geq 0$$

であるから （↪ 付録，式 (A.27)），$\lambda \geq 0$ である．同様に，$\boldsymbol{A}^\top\boldsymbol{A}$ が固有値 λ'，固有ベクトル $\boldsymbol{v}$ $(\neq \boldsymbol{0})$ を持つとして，$\boldsymbol{A}^\top\boldsymbol{A}\boldsymbol{v} = \lambda'\boldsymbol{v}$ の両辺と $\boldsymbol{v}$ の内積をとると，

$$\langle\boldsymbol{v}, \boldsymbol{A}^\top\boldsymbol{A}\boldsymbol{v}\rangle = \lambda'\langle\boldsymbol{v}, \boldsymbol{v}\rangle = \lambda'\|\boldsymbol{v}\|^2,$$

$$\langle\boldsymbol{v}, \boldsymbol{A}^\top\boldsymbol{A}\boldsymbol{v}\rangle = \langle\boldsymbol{A}\boldsymbol{v}, \boldsymbol{A}\boldsymbol{v}\rangle = \|\boldsymbol{A}\boldsymbol{v}\|^2 \geq 0$$

より，$\lambda' \geq 0$ である．

3.2. 前問より $\boldsymbol{A}\boldsymbol{A}^\top$ の固有値は正または零である．$\boldsymbol{A} \neq \boldsymbol{O}$ と仮定しているから，ひとつは正の固有値がある．それを σ^2 と書き，その固有ベクトルを $\boldsymbol{u}$ とする．$\boldsymbol{A}\boldsymbol{A}^\top\boldsymbol{u} = \sigma^2\boldsymbol{u}$ の両辺に $\boldsymbol{A}^\top$ を左から掛けると，

$$\boldsymbol{A}^\top\boldsymbol{A}\boldsymbol{A}^\top\boldsymbol{u} = \sigma^2\boldsymbol{A}^\top\boldsymbol{u}$$

である．$\boldsymbol{v} = \boldsymbol{A}^\top\boldsymbol{u}/\sigma$ と置くと，上式は $\boldsymbol{A}^\top\boldsymbol{A}(\sigma\boldsymbol{v}) = \sigma^3\boldsymbol{v}$，すなわち

$$\boldsymbol{A}^\top\boldsymbol{A}\boldsymbol{v} = \sigma^2\boldsymbol{v}$$

である．これは $\boldsymbol{A}^\top\boldsymbol{A}$ が固有値 σ^2，固有ベクトル $\boldsymbol{v}$ を持つことを意味する．逆に，$\boldsymbol{A}^\top\boldsymbol{A}$ が正の固有値 σ^2，固有ベクトル $\boldsymbol{v}$ を持つとして，$\boldsymbol{A}^\top\boldsymbol{A}\boldsymbol{v} = \sigma^2\boldsymbol{v}$ の両辺に左から $\boldsymbol{A}$ を掛けると，

$$\boldsymbol{A}\boldsymbol{A}^\top\boldsymbol{A}\boldsymbol{v} = \sigma^2\boldsymbol{A}\boldsymbol{v}$$

である．$\boldsymbol{u} = \boldsymbol{A}\boldsymbol{v}/\sigma$ と置くと，$\boldsymbol{A}\boldsymbol{A}^\top(\sigma\boldsymbol{u}) = \sigma^3\boldsymbol{u}$，すなわち

$$\boldsymbol{A}\boldsymbol{A}^\top\boldsymbol{u} = \sigma^2\boldsymbol{u}$$

である．これは $\boldsymbol{A}\boldsymbol{A}^\top$ が固有値 σ^2，固有ベクトル $\boldsymbol{u}$ を持つことを意味する．このように $\boldsymbol{A}^\top\boldsymbol{A}$, $\boldsymbol{A}^\top\boldsymbol{A}$ の一方に正の固有値 σ^2 があれば，それは他方の固有値でもあり，それぞれの固有ベクトルを $\boldsymbol{v}$, $\boldsymbol{u}$ とすると，

$$\boldsymbol{v} = \frac{\boldsymbol{A}^\top\boldsymbol{u}}{\sigma}, \qquad \boldsymbol{u} = \frac{\boldsymbol{A}\boldsymbol{v}}{\sigma}$$

が成り立つ．すなわち，式 (3.1) が成り立つ．

3.3. 次のように示せる．

(1) $\boldsymbol{A}\boldsymbol{A}^\top\boldsymbol{u} = \boldsymbol{0}$ であれば，両辺と $\boldsymbol{u}$ との内積をとると，

$$\langle \boldsymbol{u}, \boldsymbol{A}\boldsymbol{A}^\top\boldsymbol{u}\rangle = \langle \boldsymbol{A}^\top\boldsymbol{u}, \boldsymbol{A}^\top\boldsymbol{u}\rangle = \|\boldsymbol{A}^\top\boldsymbol{u}\|^2 = 0$$

となる（↪ 式 (A.27)）．ゆえに $\boldsymbol{A}^\top\boldsymbol{u} = \boldsymbol{0}$ である．

(2) $\boldsymbol{A}^\top\boldsymbol{u} = \boldsymbol{0}$ であれば，両辺と $\boldsymbol{v}$ との内積をとると

$$\langle \boldsymbol{v}, \boldsymbol{A}^\top\boldsymbol{A}\boldsymbol{v}\rangle = \langle \boldsymbol{A}\boldsymbol{v}, \boldsymbol{A}\boldsymbol{v}\rangle = \|\boldsymbol{A}\boldsymbol{v}\|^2 = 0$$

となる（↪ 式 (A.27)）．ゆえに $\boldsymbol{A}\boldsymbol{v} = \boldsymbol{0}$ である．

3.4. $\{\boldsymbol{u}_i\}$, $i = 1, ..., r$ が正規直交系であるから，行列の積の約束から，次のように計算される．

$$\boldsymbol{U}^\top\boldsymbol{U} = \begin{pmatrix} \boldsymbol{u}_1^\top \\ \vdots \\ \boldsymbol{u}_r^\top \end{pmatrix} \begin{pmatrix} \boldsymbol{u}_1 & \cdots & \boldsymbol{u}_r \end{pmatrix} = \begin{pmatrix} \langle \boldsymbol{u}_1, \boldsymbol{u}_1\rangle & \cdots & \langle \boldsymbol{u}_1, \boldsymbol{u}_r\rangle \\ \vdots & \ddots & \vdots \\ \langle \boldsymbol{u}_r, \boldsymbol{u}_1\rangle & \cdots & \langle \boldsymbol{u}_r, \boldsymbol{u}_r\rangle \end{pmatrix} = \boldsymbol{I}$$

同様に，$\{\boldsymbol{v}_i\}$, $i = 1, ..., r$ が正規直交系であるから，次のように計算される．

$$\boldsymbol{V}^\top\boldsymbol{V} = \begin{pmatrix} \boldsymbol{v}_1^\top \\ \vdots \\ \boldsymbol{v}_r^\top \end{pmatrix} \begin{pmatrix} \boldsymbol{v}_1 & \cdots & \boldsymbol{v}_r \end{pmatrix} = \begin{pmatrix} \langle \boldsymbol{v}_1, \boldsymbol{v}_1\rangle & \cdots & \langle \boldsymbol{v}_1, \boldsymbol{v}_r\rangle \\ \vdots & \ddots & \vdots \\ \langle \boldsymbol{v}_r, \boldsymbol{v}_1\rangle & \cdots & \langle \boldsymbol{v}_r, \boldsymbol{v}_r\rangle \end{pmatrix} = \boldsymbol{I}$$

3.5. 式 (2.19) より，次のように書ける．

$$\boldsymbol{U}\boldsymbol{U}^\top = \begin{pmatrix} \boldsymbol{u}_1 & \cdots & \boldsymbol{u}_r \end{pmatrix} \begin{pmatrix} \boldsymbol{u}_1^\top \\ \vdots \\ \boldsymbol{u}_r^\top \end{pmatrix} = \sum_{i=1}^{r} \boldsymbol{u}_i\boldsymbol{u}_i^\top = \boldsymbol{P}_{\mathcal{U}}$$

同様に，次のように書ける．

$$\boldsymbol{V}\boldsymbol{V}^\top = \begin{pmatrix} \boldsymbol{u}_1 & \cdots & \boldsymbol{u}_r \end{pmatrix} \begin{pmatrix} \boldsymbol{v}_1^\top \\ \vdots \\ \boldsymbol{v}_r^\top \end{pmatrix} = \sum_{i=1}^{r} \boldsymbol{v}_i\boldsymbol{v}_i^\top = \boldsymbol{P}_{\mathcal{V}}$$

第 4 章

4.1. 次のように示される．

$$\begin{aligned} \boldsymbol{A}^-\boldsymbol{A} &= \Big(\sum_{i=1}^{n} \frac{\boldsymbol{v}_i\boldsymbol{u}_i^\top}{\sigma_i}\Big)\Big(\sum_{j=1}^{n} \sigma_j\boldsymbol{u}_j\boldsymbol{v}_j^\top\Big) = \sum_{i,j=1}^{n} \frac{\sigma_i}{\sigma_j}\boldsymbol{v}_i\boldsymbol{u}_i^\top\boldsymbol{u}_j\boldsymbol{v}_j^\top = \sum_{i,j=1}^{n} \frac{\sigma_i}{\sigma_j}\boldsymbol{v}_i\langle \boldsymbol{u}_i, \boldsymbol{u}_j\rangle\boldsymbol{v}_j^\top \\ &= \sum_{i,j=1}^{n} \frac{\sigma_i}{\sigma_j}\delta_{ij}\boldsymbol{v}_i\boldsymbol{v}_j^\top = \sum_{i=1}^{n} \boldsymbol{v}_i\boldsymbol{v}_j^\top = \boldsymbol{I} \end{aligned}$$

積が単位行列であるから，$\boldsymbol{A}^-$ は $\boldsymbol{A}$ の逆行列である．

4.2. 次の関係が成り立つ．

$$\begin{aligned}\boldsymbol{A}\boldsymbol{A}^{-} &= \boldsymbol{U}\begin{pmatrix}\sigma_1 & & \\ & \ddots & \\ & & \sigma_r\end{pmatrix}\boldsymbol{V}^{\top}\boldsymbol{V}\begin{pmatrix}1/\sigma_1 & & \\ & \ddots & \\ & & 1/\sigma_r\end{pmatrix}\boldsymbol{U}^{\top} \\ &= \boldsymbol{U}\begin{pmatrix}\sigma_1 & & \\ & \ddots & \\ & & \sigma_r\end{pmatrix}\begin{pmatrix}1/\sigma_1 & & \\ & \ddots & \\ & & 1/\sigma_r\end{pmatrix}\boldsymbol{U}^{\top} = \boldsymbol{U}\boldsymbol{U}^{\top} = \boldsymbol{P}_{\mathcal{U}}\end{aligned}$$

ただし，式 (3.12), (3.13) を用いた．同様に，次の関係が成り立つ．

$$\begin{aligned}\boldsymbol{A}^{-}\boldsymbol{A} &= \boldsymbol{V}\begin{pmatrix}1/\sigma_1 & & \\ & \ddots & \\ & & 1/\sigma_r\end{pmatrix}\boldsymbol{U}^{\top}\boldsymbol{U}\begin{pmatrix}\sigma_1 & & \\ & \ddots & \\ & & \sigma_r\end{pmatrix}\boldsymbol{V}^{\top} \\ &= \boldsymbol{V}\begin{pmatrix}1/\sigma_1 & & \\ & \ddots & \\ & & 1/\sigma_r\end{pmatrix}\begin{pmatrix}\sigma_1 & & \\ & \ddots & \\ & & \sigma_r\end{pmatrix}\boldsymbol{V}^{\top} = \boldsymbol{V}\boldsymbol{V}^{\top} = \boldsymbol{P}_{\mathcal{V}}\end{aligned}$$

4.3. 次のように示される．

$$\begin{aligned}\boldsymbol{A}^{-}\boldsymbol{A}\boldsymbol{A}^{-} &= \boldsymbol{V}\begin{pmatrix}1/\sigma_1 & & \\ & \ddots & \\ & & 1/\sigma_r\end{pmatrix}\boldsymbol{U}^{\top}\boldsymbol{U}\begin{pmatrix}\sigma_1 & & \\ & \ddots & \\ & & \sigma_r\end{pmatrix}\boldsymbol{V}^{\top}\boldsymbol{V}\begin{pmatrix}1/\sigma_1 & & \\ & \ddots & \\ & & 1/\sigma_r\end{pmatrix}\boldsymbol{U}^{\top} \\ &= \boldsymbol{V}\begin{pmatrix}1/\sigma_1 & & \\ & \ddots & \\ & & 1/\sigma_r\end{pmatrix}\begin{pmatrix}\sigma_1 & & \\ & \ddots & \\ & & \sigma_r\end{pmatrix}\begin{pmatrix}1/\sigma_1 & & \\ & \ddots & \\ & & 1/\sigma_r\end{pmatrix}\boldsymbol{U}^{\top} \\ &= \boldsymbol{V}\begin{pmatrix}1/\sigma_1 & & \\ & \ddots & \\ & & 1/\sigma_r\end{pmatrix}\boldsymbol{U}^{\top} = \boldsymbol{A}^{-}\end{aligned}$$

ただし，式 (3.12) を用いた．同様にして次式も得られる．

$$\begin{aligned}\boldsymbol{A}\boldsymbol{A}^{-}\boldsymbol{A} &= \boldsymbol{U}\begin{pmatrix}\sigma_1 & & \\ & \ddots & \\ & & \sigma_r\end{pmatrix}\boldsymbol{V}^{\top}\boldsymbol{V}\begin{pmatrix}1/\sigma_1 & & \\ & \ddots & \\ & & 1/\sigma_r\end{pmatrix}\boldsymbol{U}^{\top}\boldsymbol{U}\begin{pmatrix}\sigma_1 & & \\ & \ddots & \\ & & \sigma_r\end{pmatrix}\boldsymbol{V}^{\top}\boldsymbol{V} \\ &= \boldsymbol{U}\begin{pmatrix}\sigma_1 & & \\ & \ddots & \\ & & \sigma_r\end{pmatrix}\begin{pmatrix}1/\sigma_1 & & \\ & \ddots & \\ & & 1/\sigma_r\end{pmatrix}\begin{pmatrix}\sigma_1 & & \\ & \ddots & \\ & & \sigma_r\end{pmatrix}\boldsymbol{V}^{\top} \\ &= \boldsymbol{U}\begin{pmatrix}\sigma_1 & & \\ & \ddots & \\ & & \sigma_r\end{pmatrix}\boldsymbol{V}^{\top} = \boldsymbol{A}\end{aligned}$$

4.4. $\boldsymbol{A} = \Big(A_{ij}\Big)$, $\boldsymbol{B} = \Big(B_{ij}\Big)$ に対して，$\boldsymbol{A}\boldsymbol{B}$, $\boldsymbol{B}\boldsymbol{A}$ の (i,j) 要素は，それぞれ $\sum_k A_{ik}B_{kj}$, $\sum_k B_{ik}A_{kj}$ である．それらのトレースは $\sum_{j,k} A_{jk}B_{kj}$, $\sum_{j,k} B_{jk}A_{kj}$ であり，等しい．

4.5. 次のように示される．

$$\begin{aligned}\|\boldsymbol{AU}\|^2 &= \mathrm{tr}(\boldsymbol{AU}(\boldsymbol{AU})^\top) = \mathrm{tr}(\boldsymbol{AUU}^\top\boldsymbol{A}^\top) = \mathrm{tr}(\boldsymbol{AA}^\top) = \|\boldsymbol{A}\|^2\\ \|\boldsymbol{VA}\|^2 &= \mathrm{tr}((\boldsymbol{VA})^\top\boldsymbol{VA}) = \mathrm{tr}(\boldsymbol{A}^\top\boldsymbol{VVA}) = \mathrm{tr}(\boldsymbol{A}^\top\boldsymbol{A}) = \|\boldsymbol{A}\|^2\\ \|\boldsymbol{VAU}\|^2 &= \mathrm{tr}(\boldsymbol{VAU}(\boldsymbol{VAU})^\top) = \mathrm{tr}(\boldsymbol{VAUU}^\top\boldsymbol{A}^\top\boldsymbol{V}^\top) = \mathrm{tr}(\boldsymbol{VAA}^\top\boldsymbol{V}^\top)\\ &= \mathrm{tr}(\boldsymbol{V}^\top\boldsymbol{VAA}^\top) = \mathrm{tr}(\boldsymbol{AA}^\top) = \|\boldsymbol{A}\|^2\end{aligned}$$

ただし，式 (4.21)，および $\boldsymbol{U}$, $\boldsymbol{V}$ が直交行列であり，$\boldsymbol{U}^\top\boldsymbol{U} = \boldsymbol{UU}^\top = \boldsymbol{I}$, $\boldsymbol{V}^\top\boldsymbol{V} = \boldsymbol{VV}^\top = \boldsymbol{I}$ であることを用いた．

4.6. 式 (3.10) から，次式が成り立つ．

$$\begin{aligned}\|\boldsymbol{A}\|^2 &= \mathrm{tr}(\boldsymbol{AA}^\top) = \mathrm{tr}(\boldsymbol{U}\begin{pmatrix}\sigma_1 & & \\ & \ddots & \\ & & \sigma_r\end{pmatrix}\boldsymbol{V}^\top\boldsymbol{V}\begin{pmatrix}\sigma_1 & & \\ & \ddots & \\ & & \sigma_r\end{pmatrix}\boldsymbol{U}^\top)\\ &= \mathrm{tr}(\boldsymbol{U}\begin{pmatrix}\sigma_1 & & \\ & \ddots & \\ & & \sigma_r\end{pmatrix}\begin{pmatrix}\sigma_1 & & \\ & \ddots & \\ & & \sigma_r\end{pmatrix}\boldsymbol{U}^\top) = \mathrm{tr}(\boldsymbol{U}\begin{pmatrix}\sigma_1^2 & & \\ & \ddots & \\ & & \sigma_r^2\end{pmatrix}\boldsymbol{U}^\top)\\ &= \mathrm{tr}(\boldsymbol{U}^\top\boldsymbol{U}\begin{pmatrix}\sigma_1^2 & & \\ & \ddots & \\ & & \sigma_r^2\end{pmatrix}) = \mathrm{tr}(\begin{pmatrix}\sigma_1^2 & & \\ & \ddots & \\ & & \sigma_r^2\end{pmatrix}) = \sigma_1^2 + \cdots + \sigma_r^2\end{aligned}$$

ただし，$\boldsymbol{U}$, $\boldsymbol{V}$ は必ずしも直交行列ではないが（正方行列とは限らない），式 (3.12) が成り立つことを用いた．この結果を用いると，式 (4.14) と (4.16) から

$$\boldsymbol{A} - (\boldsymbol{A})_r = \boldsymbol{U}\begin{pmatrix}0 & & & & & \\ & \ddots & & & & \\ & & 0 & & & \\ & & & \sigma_{r+1} & & \\ & & & & \ddots & \\ & & & & & \sigma_l\end{pmatrix}\boldsymbol{V}^\top$$

であるから，式 (4.20) が得られる．

第 5 章

5.1. (1) 式 (5.5) は次のように書ける．

$$J = \langle \boldsymbol{Ax} - \boldsymbol{b}, \boldsymbol{Ax} - \boldsymbol{b}\rangle = \langle \boldsymbol{Ax}, \boldsymbol{Ax}\rangle - 2\langle \boldsymbol{Ax}, \boldsymbol{b}\rangle + \langle \boldsymbol{b}, \boldsymbol{b}\rangle = \langle \boldsymbol{x}, \boldsymbol{A}^\top\boldsymbol{Ax}\rangle - 2\langle \boldsymbol{x}, \boldsymbol{A}^\top\boldsymbol{b}\rangle + \|\boldsymbol{b}\|^2$$

これを $\boldsymbol{x}$ で微分して $\boldsymbol{0}$ と置くと（↪ 付録，式 (A.15), (A.25) ），次式を得る．

$$2\boldsymbol{A}^\top\boldsymbol{Ax} - 2\boldsymbol{A}^\top\boldsymbol{b} = \boldsymbol{0}$$

$m > n$ であり，$r = n$ であれば，$\boldsymbol{A}^\top\boldsymbol{A}$ は $n \times n$ 正則行列である．ゆえに，解 $\boldsymbol{x}$ が式 (5.24) で与えられる．

(2) 上記の J の式中の $\boldsymbol{A}^\top\boldsymbol{Ax}$ を $\boldsymbol{A}^\top\boldsymbol{b}$ で置き換えると，J は次のように書ける．

$$J = \langle \boldsymbol{x}, \boldsymbol{A}^\top\boldsymbol{b}\rangle - 2\langle \boldsymbol{x}, \boldsymbol{A}^\top\boldsymbol{b}\rangle + \|\boldsymbol{b}\|^2 = \|\boldsymbol{b}\|^2 - \langle \boldsymbol{x}, \boldsymbol{A}^\top\boldsymbol{b}\rangle$$

5.2. $\boldsymbol{A}$ が式 (3.4) のように特異値分解されているとき，次式が成り立つ．

$$\begin{aligned}\boldsymbol{A}^\top\boldsymbol{A} &= \Big(\sum_{i=1}^r \sigma_i\boldsymbol{v}_i\boldsymbol{u}_i^\top\Big)\Big(\sum_{j=1}^r \sigma_j\boldsymbol{u}_j\boldsymbol{v}_j^\top\Big) = \sum_{i,j=1}^r \sigma_i\sigma_j\boldsymbol{v}_i\boldsymbol{u}_i^\top\boldsymbol{u}_j\boldsymbol{v}_j^\top = \sum_{i,j=1}^r \sigma_i\sigma_j\boldsymbol{v}_i\langle\boldsymbol{u}_i,\boldsymbol{u}_j\rangle\boldsymbol{v}_j^\top \\ &= \sum_{i,j=1}^r \delta_{ij}\sigma_i\sigma_j\boldsymbol{v}_i\boldsymbol{v}_j^\top = \sum_{i=1}^r \sigma_i^2\boldsymbol{v}_i\boldsymbol{v}_i^\top\end{aligned}$$

$$\begin{aligned}(\boldsymbol{A}^\top\boldsymbol{A})^{-1}\boldsymbol{A}^\top &= \Big(\sum_{i=1}^r \frac{\boldsymbol{v}_i\boldsymbol{v}_i^\top}{\sigma_i^2}\Big)\Big(\sum_{j=1}^r \sigma_j\boldsymbol{v}_j\boldsymbol{u}_j^\top\Big) = \sum_{i,j=1}^r \frac{\sigma_j}{\sigma_i^2}\boldsymbol{v}_i\boldsymbol{v}_i^\top\boldsymbol{v}_j\boldsymbol{u}_j^\top = \sum_{i,j=1}^r \frac{\sigma_j}{\sigma_i^2}\boldsymbol{v}_i\langle\boldsymbol{v}_i,\boldsymbol{v}_j\rangle\boldsymbol{u}_j^\top \\ &= \sum_{i,j=1}^r \frac{\sigma_j}{\sigma_i^2}\delta_{ij}\boldsymbol{v}_i\boldsymbol{u}_j^\top = \sum_{i=1}^r \frac{\boldsymbol{v}_i\boldsymbol{u}_i^\top}{\sigma_i} = \boldsymbol{A}^-\end{aligned}$$

5.3. $\|\boldsymbol{x}\|^2/2$ を条件 $\boldsymbol{A}\boldsymbol{x} = \boldsymbol{b}$ のもとで最小化する（1/2 は形式的なもので，特に意味はない）．ラグランジュ乗数 $\boldsymbol{\lambda}$（↪ 付録，式 (A.48)）を導入して，

$$\frac{1}{2}\|\boldsymbol{x}\|^2 - \langle\boldsymbol{\lambda},\boldsymbol{A}\boldsymbol{x}-\boldsymbol{b}\rangle = \frac{1}{2}\langle\boldsymbol{x},\boldsymbol{x}\rangle - \langle\boldsymbol{A}^\top\boldsymbol{\lambda},\boldsymbol{x}\rangle + \langle\boldsymbol{\lambda},\boldsymbol{b}\rangle$$

を $\boldsymbol{x}$ で微分して $\boldsymbol{0}$ と置くと（↪ 付録，式 (A.15), (A.25) ），次式を得る．

$$\boldsymbol{x} - \boldsymbol{A}^\top\boldsymbol{\lambda} = \boldsymbol{0}$$

したがって，$\boldsymbol{A}\boldsymbol{x} = \boldsymbol{b}$ は次のように書ける．

$$\boldsymbol{A}\boldsymbol{A}^\top\boldsymbol{\lambda} = \boldsymbol{b}$$

$m < n$ であり，$r = m$ であれば，$\boldsymbol{A}\boldsymbol{A}^\top$ は $m \times m$ 正則行列である．ゆえに，$\boldsymbol{\lambda}$ が次のように与えられる．

$$\boldsymbol{\lambda} = (\boldsymbol{A}\boldsymbol{A}^\top)^{-1}\boldsymbol{b}$$

したがって，$\boldsymbol{x}$ が次のように表せる．

$$\boldsymbol{x} = \boldsymbol{A}^\top\boldsymbol{\lambda} = \boldsymbol{A}(\boldsymbol{A}\boldsymbol{A}^\top)^{-1}\boldsymbol{b}$$

$\boldsymbol{A}\boldsymbol{x} = \boldsymbol{b}$ が満たされているから，$J = \|\boldsymbol{A}\boldsymbol{x}-\boldsymbol{b}\|^2 = 0$ である．

5.4. $\boldsymbol{A}$ が式 (3.4) のように特異値分解されているとき，次式が成り立つ．

$$\begin{aligned}\boldsymbol{A}\boldsymbol{A}^\top &= \Big(\sum_{i=1}^r \sigma_i\boldsymbol{u}_i\boldsymbol{v}_i^\top\Big)\Big(\sum_{j=1}^r \sigma_j\boldsymbol{v}_j\boldsymbol{u}_j^\top\Big) = \sum_{i,j=1}^r \sigma_i\sigma_j\boldsymbol{u}_i\boldsymbol{v}_i^\top\boldsymbol{v}_j\boldsymbol{u}_j^\top = \sum_{i,j=1}^r \sigma_i\sigma_j\boldsymbol{u}_i\langle\boldsymbol{v}_i,\boldsymbol{v}_j\rangle\boldsymbol{u}_j^\top \\ &= \sum_{i,j=1}^r \delta_{ij}\sigma_i\sigma_j\boldsymbol{u}_i\boldsymbol{u}_j^\top = \sum_{i=1}^r \sigma_i^2\boldsymbol{u}_i\boldsymbol{u}_i^\top\end{aligned}$$

$$\begin{aligned}\boldsymbol{A}^\top(\boldsymbol{A}\boldsymbol{A}^\top)^{-1} &= \Big(\sum_{i=1}^r \sigma_i\boldsymbol{v}_i\boldsymbol{u}_i^\top\Big)\Big(\sum_{j=1}^r \frac{\boldsymbol{u}_j\boldsymbol{u}_j^\top}{\sigma_j^2}\Big) = \sum_{i,j=1}^r \frac{\sigma_i}{\sigma_j^2}\boldsymbol{v}_i\boldsymbol{u}_i^\top\boldsymbol{u}_j\boldsymbol{u}_j^\top = \sum_{i,j=1}^r \frac{\sigma_i}{\sigma_j^2}\boldsymbol{v}_i\langle\boldsymbol{u}_i,\boldsymbol{u}_j\rangle\boldsymbol{u}_j^\top \\ &= \sum_{i,j=1}^r \frac{\sigma_i}{\sigma_j^2}\delta_{ij}\boldsymbol{v}_i\boldsymbol{u}_j^\top = \sum_{i=1}^r \frac{\boldsymbol{v}_i\boldsymbol{u}_i^\top}{\sigma_i} = \boldsymbol{A}^-\end{aligned}$$

5.5. 式 (5.19) を x で微分すると，次のようになる．

$$\frac{dJ}{dx} = 2(a_1x - b_1)a_1 + \cdots + 2(a_mx - b_m)a_m = 2(a_1^1 + \cdots + a_m^2)x - 2(a_1b_1 + \cdots + a_mb_m)$$

これを 0 と置くと，式 (5.17) が得られる．

5.6. $\|\boldsymbol{x}\|^2/2$ を式 (5.20) の制約のもとで最小化する（1/2 は形式的なもので，特に意味はない）．ラグランジュ乗数 λ（↪ 付録，式 (A.46)）を導入して，

$$\frac{1}{2}\|\boldsymbol{x}\|^2 - \lambda(\langle \boldsymbol{a}, \boldsymbol{x}\rangle - b)$$

を $\boldsymbol{x}$ で微分して $\boldsymbol{0}$ と置くと（↪ 付録，式 (A.15), (A.25) ），次式を得る．

$$\boldsymbol{x} - \lambda\boldsymbol{a} = \boldsymbol{0}$$

すなわち，$\boldsymbol{x} = \lambda\boldsymbol{a}$ である．これを $\langle \boldsymbol{a}, \boldsymbol{x}\rangle = b$ に代入すると，

$$\lambda\|\boldsymbol{a}\|^2 = b$$

となり，$\lambda = b/\|\boldsymbol{a}\|^2$ である．したがって，

$$\boldsymbol{x} = \frac{b\boldsymbol{a}}{\|\boldsymbol{a}\|^2}$$

が得られる．

第 6 章

6.1. 定義より，$\boldsymbol{\Sigma}$ の (i, i) 要素 $E[\Delta x_i^2] = E[(x_i - \bar{x}_i)^2]$ は x_i の分散である（x_i の期待値を $\bar{x}_i = 0$ と仮定していることに注意）．そして，非対角要素 $E[\Delta x_i \Delta x_j] = E[(x_i - \bar{x}_i)(x_j - \bar{x}_j)]$ は x_i, x_j の共分散である．

6.2. 明らかに $\boldsymbol{X}$ は対称行列である：$\boldsymbol{X}^\top = \boldsymbol{x}\boldsymbol{x}^\top = (\boldsymbol{x}^\top)^\top\boldsymbol{x}^\top = \boldsymbol{X}$．その固有値を σ，固有ベクトルを $\boldsymbol{u}$ とし，$\boldsymbol{X}\boldsymbol{u} = \sigma\boldsymbol{u}$ の両辺と $\boldsymbol{u}$ との内積をとると，

$$\langle \boldsymbol{u}, \boldsymbol{X}\boldsymbol{u}\rangle = \sigma\langle \boldsymbol{u}, \boldsymbol{u}\rangle = \sigma\|\boldsymbol{u}\|^2$$

であるが，

$$\langle \boldsymbol{u}, \boldsymbol{X}\boldsymbol{u}\rangle = \langle \boldsymbol{u}, \boldsymbol{x}\boldsymbol{x}^\top\boldsymbol{u}\rangle = \langle \boldsymbol{u}, \boldsymbol{x}\rangle\langle \boldsymbol{x}, \boldsymbol{u}\rangle = \langle \boldsymbol{u}, \boldsymbol{x}\rangle^2 \geq 0$$

であるから，$\sigma \geq 0$ である．複数のベクトルに対しても，

$$\langle \boldsymbol{u}, \boldsymbol{X}\boldsymbol{u}\rangle = \langle \boldsymbol{u}, \sum_{\alpha=1}^{N} \boldsymbol{x}_\alpha\boldsymbol{x}_\alpha^\top\boldsymbol{u}\rangle = \sum_{\alpha=1}^{N}\langle \boldsymbol{u}, \boldsymbol{x}_\alpha\boldsymbol{x}_\alpha^\top\boldsymbol{u}\rangle = \sum_{\alpha=1}^{N}\langle \boldsymbol{u}, \boldsymbol{x}_\alpha\rangle\langle \boldsymbol{x}_\alpha, \boldsymbol{u}\rangle = \sum_{\alpha=1}^{N}\langle \boldsymbol{u}, \boldsymbol{x}_\alpha\rangle^2 \geq 0$$

であるから，$\sigma \geq 0$ である．

6.3. 式 (1.23) より，$\mathrm{tr}(\boldsymbol{x}\boldsymbol{x}^\top) = \langle \boldsymbol{x}, \boldsymbol{x}\rangle = \|\boldsymbol{x}\|^2$ である．ゆえに $\mathrm{tr}(\sum_{\alpha=1}^{N} \boldsymbol{x}_\alpha\boldsymbol{x}_\alpha^\top) = \sum_{\alpha=1}^{N} \|\boldsymbol{x}_\alpha\|^2$ である．

6.4. 3 次元空間において $\boldsymbol{\Sigma} = \mathrm{diag}(\sigma_1^2, \sigma_2^2, \sigma_3^2)$, $\sigma_1^2, \sigma_2^2, \sigma_3^2 > 0$ とすると（$\mathrm{diag}(\cdots)$ は $\cdots$ をその順に対角要素とする対角行列を表す），その逆行列は $\boldsymbol{\Sigma}^{-1} = \mathrm{diag}(1/\sigma_1^2, 1/\sigma_2^2, 1/\sigma_3^2)$ である．ゆえに，式 (6.10) は次のように書ける．

$$\frac{(x - \bar{x})^2}{\sigma_1^2} + \frac{(y - \bar{y})^2}{\sigma_2^2} + \frac{(z - \bar{z})^2}{\sigma_3^2} = 1$$

これは $(\bar{x}, \bar{y}, \bar{z})$ を中心として，各座標軸を対称軸とし，x, y, z 軸方向の半径がそれぞれ σ_1, σ_2, σ_3 の楕円体である．

6.5. 共分散行列 $\boldsymbol{\Sigma}$ が正値のとき，これは $\boldsymbol{\Sigma} = \sum_{i=1}^{n} \sigma_i^2 \boldsymbol{u}_i \boldsymbol{u}_i^\top$, $\sigma_i^2 > 0$, $i = 1, ..., n$ とスペクトル分解できる．座標系を $\bar{\boldsymbol{x}}$ が原点 O になるよう平行移動し，その周りに，座標軸が $\boldsymbol{\Sigma}$ の固有ベクトル $\boldsymbol{u}_1, ..., \boldsymbol{u}_n$ の方向に一致するように回転する．この新しい座標系では共分散行列は $\boldsymbol{\Sigma} = \mathrm{diag}(\sigma_1^2, ..., \sigma_n^2)$ となり，その逆行列は $\boldsymbol{\Sigma}^{-1} = \mathrm{diag}(1/\sigma_1^2, ..., 1/\sigma_n^2)$ である．ゆえに，式 (6.10) は

$$\frac{x_1^2}{\sigma_1^2} + \cdots + \frac{x_n^2}{\sigma_n^2} = 1$$

と書ける．これは原点を中心とし，各座標軸が対称軸で，各軸方向の半径が σ_i の楕円体を表す．もとの座標系では，これは期待値 $\bar{\boldsymbol{x}}$ を中心とし，$\boldsymbol{\Sigma}$ の各固有ベクトル $\boldsymbol{u}_i$ が対称軸で，各軸方向の半径が σ_i の楕円体である．

6.6. 定義より，$\boldsymbol{S}$ の (i, i) 要素

$$S_{ii} = \frac{1}{N} \sum_{\alpha=1}^{N} (\hat{x}_{i\alpha} - m_i)^2$$

は $x_{i\alpha}$ のサンプル分散である．ただし，

$$m_i = \frac{1}{N} \sum_{\alpha=1}^{N} \hat{x}_{i\alpha}$$

は $x_{i\alpha}$ のサンプル平均である．そして，非対角要素

$$S_{ij} = \frac{1}{N} \sum_{\alpha=1}^{N} (\hat{x}_{i\alpha} - m_i)(\hat{x}_{j\alpha} - m_j)$$

は $x_{i\alpha}$, $x_{j\alpha}$ の共分散である．

第 7 章

7.1. $\boldsymbol{A}$ のスペクトル分解を $\boldsymbol{A} = \sum_{i=1}^{n} \lambda_i \boldsymbol{u}_i \boldsymbol{u}_i^\top$ とすると，次のようになる．

$$\mathrm{tr}\boldsymbol{A} = \sum_{i=1}^{n} \lambda_i \mathrm{tr}(\boldsymbol{u}_i \boldsymbol{u}_i^\top) = \sum_{i=1}^{n} \lambda_i \|\boldsymbol{u}_i\|^2 = \sum_{i=1}^{n} \lambda_i$$

7.2. $\boldsymbol{x}_0$ を基準にとって，$\boldsymbol{x}_0$ を原点とみなすと，残りの n 本のベクトルが線形独立である条件は次のように書ける．

$$\left| \begin{array}{ccc} \boldsymbol{x}_1 - \boldsymbol{x}_0 & \cdots & \boldsymbol{x}_n - \boldsymbol{x}_0 \end{array} \right| \neq 0$$

左辺の $n \times n$ 行列の行列式は，次の $(n+1) \times (n+1)$ 行列の行列式に等しい．

$$\left| \begin{array}{ccccc} \boldsymbol{x}_0 & \boldsymbol{x}_1 - \boldsymbol{x}_0 & \cdots & \boldsymbol{x}_n - \boldsymbol{x}_0 \\ 1 & 0 & \cdots & 0 \end{array} \right| = \left| \begin{array}{ccccc} \boldsymbol{x}_0 & \boldsymbol{x}_1 & \cdots & \boldsymbol{x}_n \\ 1 & 1 & \cdots & 1 \end{array} \right|$$

ただし，第 1 列を他の列に加えた（それによって行列式は変化しない）．これは $\boldsymbol{x}_0$ を基準にとったものであるが，どの $\boldsymbol{x}_i$ を基準にとっても同じ表現が得られる．

7.3. $J = \sum_{\alpha=1}^{N} \|\boldsymbol{x}_\alpha - \boldsymbol{g}\|^2 = \sum_{\alpha=1}^{N} (\boldsymbol{x}_\alpha - \boldsymbol{g}, \boldsymbol{x}_\alpha - \boldsymbol{g})$ を $\boldsymbol{x}$ で微分すると（↪ 付録，式 (A.15), (A.25) ），$\nabla J = 2 \sum_{\alpha=1}^{N} (\boldsymbol{x}_\alpha - \boldsymbol{g}) = 2 \sum_{\alpha=1}^{N} \boldsymbol{x}_\alpha - 2N\boldsymbol{g}$ である．これを $\boldsymbol{0}$ と置くと．式 (7.13) が得られる．

7.4. $\sum_{\alpha=1}^{N} \boldsymbol{x}_\alpha = N\boldsymbol{g}$ より，次のように示せる．

$$\begin{aligned} \boldsymbol{\Sigma} &= \sum_{\alpha=1}^{N} (\boldsymbol{x}_\alpha - \boldsymbol{g})(\boldsymbol{x}_\alpha - \boldsymbol{g})^\top = \sum_{\alpha=1}^{N} \boldsymbol{x}_\alpha \boldsymbol{x}_\alpha^\top - \sum_{\alpha=1}^{N} \boldsymbol{x}_\alpha \boldsymbol{g}^\top - \sum_{\alpha=1}^{N} \boldsymbol{g} \boldsymbol{x}_\alpha^\top + \sum_{\alpha=1}^{N} \boldsymbol{g}\boldsymbol{g}^\top \\ &= \sum_{\alpha=1}^{N} \boldsymbol{x}_\alpha \boldsymbol{x}_\alpha^\top - N\boldsymbol{g}\boldsymbol{g}^\top - N\boldsymbol{g}\boldsymbol{g}^\top + N\boldsymbol{g}\boldsymbol{g}^\top = \sum_{\alpha=1}^{N} \boldsymbol{x}_\alpha \boldsymbol{x}_\alpha^\top - N\boldsymbol{g}\boldsymbol{g}^\top \end{aligned}$$

第 8 章

8.1. $\boldsymbol{A}$ がランク r 以下であれば，式 (8.4) – (8.6) のようにして，ある $m \times r$ 行列 $\boldsymbol{A}_1$ とある $r \times n$ 行列 $\boldsymbol{A}_2$ によっ て，$\boldsymbol{A} = \boldsymbol{A}_1\boldsymbol{A}_2$ と分解できる．逆に，ある $m \times r$ 行列 $\boldsymbol{A}_1$ とある $r \times n$ 行列 $\boldsymbol{A}_2$ によっつて $\boldsymbol{A} = \boldsymbol{A}_1\boldsymbol{A}_2$ と分解できていれば，式 (8.3) より $\boldsymbol{A}$ はランク r 以下である．

8.2. (1) 式 (8.11) の $2M$ 運動行列 $\boldsymbol{M}$ の 3 本の列を $\boldsymbol{m}_1$, $\boldsymbol{m}_2$, $\boldsymbol{m}_3$ とすると，式 (8.12) は，式 (8.10) の第 α 列が次のように書けることを意味する．

$$\begin{pmatrix} x_{\alpha 1} \\ y_{\alpha 2} \\ \cdots \\ x_{\alpha M} \\ y_{\alpha M} \end{pmatrix} = X_\alpha \boldsymbol{m}_1 + Y_\alpha \boldsymbol{m}_2 + Z_\alpha \boldsymbol{m}_3$$

これは，第 α 点の軌跡が $\boldsymbol{m}_1$, $\boldsymbol{m}_2$, $\boldsymbol{m}_3$ の張る 3 次元部分空間に含まれていることを意味する．したがって，どの点の軌跡もこの 3 次元部分空間に含まれる．

(2) この 3 次元部分空間を求めることは，$2M$ 次元空間の N 点 $(x_{\alpha 1}, y_{\alpha 2}, ..., x_{\alpha M}, y_{\alpha M})$, $\alpha = 1, ..., N$ に 3 次元部分空間を当てはめる問題となる．したがって，7.3 節で述べたように，この N 点を列として並べた $2M \times N$ 行列，すなわち，式 (8.10) の観測行列 $\boldsymbol{W}$ を

$$\boldsymbol{W} = \sigma_1 \boldsymbol{u}_1 \boldsymbol{v}_1 + \sigma_2 \boldsymbol{u}_2 \boldsymbol{v}_2 + \sigma_3 \boldsymbol{u}_3 \boldsymbol{v}_3 + \cdots$$

と特異値分解すれば，$\{\boldsymbol{u}_1, \boldsymbol{u}_2, \boldsymbol{u}_3\}$ がその 3 次元部分空間の正値直交基底である．このとき，仮想敵なカメラ（アフィンカメラ）では式 (8.12) の分解が成り立って，$\boldsymbol{W}$ ランクが 3 であり，$\sigma_4 = \sigma_5 = \cdots = 0$ であるが，実際のカメラから得た観測行列 $\boldsymbol{W}$ ではそれらは 0 でないので，最初の 3 項を取り出す．これが最適な当てはめである．