Session 1. (1) Principal component analysis and Karhunen-Loève transformation

Topic 2 of this course explains the image compression by orthogonal transformations. This method expresses an image by a weighted summation of "something," and reduce the data amount by omitting some terms in the summation. Successful data amount reduction without significant degradation of image quality should separate the terms corresponding to "visually more important components" and those corresponding to "visually less important components" in the weighted summation, and remove the latter.

This topic consists of the following three sessions; 1) Derivation of the statistically optimal weighted summation by the principal component analysis and Karhunen-Loève transformation, 2) Introduction of unitary transformations of matrices for general formalization of the KL transformation and introduction of basis images as the terms in the weighted summation, and 3) image compression using cosine transformation and JPEG method as an empirically optimal formalization of the weighted summation.

Visually "more important components" and "less important components"

We consider here an image consising of only two pixels for simplicity, and consider treating various twopixel images. It is obvious that there can be many combinations of pixel values in an image. Let the two pixel values be x_1 and x_2, and consider illustrating the distribution of the images by locating each image on $x_1 x_2-$ plane. Figure 1 is an example of the distribution, and each of symbol "+" corresponds to an image. In the case of Fig. 1, the variances of both x_1 and x_2 are large. It indicates that both coordinates have meaningful roles and neither x_1 nor x_2 can be omitted.

On the other hand, in the case of the distribution as shown in Fig. 2, the variance of x_1 is large while that of x_2 is small, i. e. x_2 does not vary very much for all images. This means that only x_1 is important for expressing the difference of the images, and that x_1 is not important and can be replaced with a constant, for example the average of x_2 for all images.

How can we create such distribution as Fig. 2 if the original distribution of images is as Fig. 1? The answer is rotating the coordinates as shown in Fig. 3. The coordinates z_1 and z_2 are created by a rotation of x_1 and x_2, respectively. The variance of z_1 is the maximum subject to all possible rotations in the case of Fig. 3. The transformed pixel value z_1 is the "most important component" and z_2 is the "less important component" in this case.

Principal component analysis

We derive the above z_1 and z_2 in the followings. We assume the relationship between z_1 and (x_1, x_2) as follows[1]:

$$z_1 = a_1 x_1 + a_2 x_2. \tag{1}$$

Let x_{1i} and x_{2i} be the values of pixels x_1 and x_2 of the ith image, respectively. The averages of x_1 and x_2, denoted $\overline{x_1}$ and $\overline{x_2}$, respectively, the variances s_{11} and s_{22}, and the covariance $s_{12} = s_{21}$ are defined as follows:

$$\overline{x_1} = \frac{1}{n}\sum_{i=1}^{n} x_{1i}, \quad \overline{x_2} = \frac{1}{n}\sum_{i=1}^{n} x_{2i}$$

$$s_{11} = \frac{1}{n}\sum_{i=1}^{n}(x_{1i} - \overline{x_1})^2, \quad s_{22} = \frac{1}{n}\sum_{i=1}^{n}(x_{2i} - \overline{x_2})^2$$

$$s_{12} = s_{21} = \frac{1}{n}\sum_{i=1}^{n}(x_{1i} - \overline{x_1})(x_{2i} - \overline{x_2}). \tag{2}$$

Dividing the covariance $s_{12} = s_{21}$ by (the standard deviation of x_1) × (the standard deviation of x_2), i. e. $\sqrt{s_{11}}\sqrt{s_{22}}$, we get the correlation coefficient. The covariance is zero if x_1 and x_2 do not correlate. This is

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[1]It is often assumed alternatively as $z_1 = a_1(x_1 - \overline{x_1}) + a_2(x_2 - \overline{x_2})$. The covariance matrices are the same as the case in the main text.

intuitively explained as follows: If we take $\overline{x_1}$ and $\overline{x_2}$ as new coordinates, $(x_{1i} - \overline{x_1})(x_{2i} - \overline{x_2})$ is positive in the first and the third quadrants, and negative in the second and the fourth quadrants. If x_1 and x_2 do not correlate, as shown in Fig. 4, positive values and negative values of the products $(x_{1i} - \overline{x_1})(x_{2i} - \overline{x_2})$ cancel each other and their summation is zero.

The variance of z_1, denoted $V(z_1)$, is derived from Eqs. (1) and (2), as follows:

$$
\begin{aligned}
V(z_1) &= \frac{1}{n} \sum_{i=1}^{n} (z_{1i} - \overline{z_1})^2 \\
&= \frac{1}{n} \sum_{i=1}^{n} \{(a_1 x_{1i} + a_2 x_{2i}) - (a_1 \overline{x_1} + a_2 \overline{x_2})\}^2 \\
&= \frac{1}{n} \sum_{i=1}^{n} \{(a_1(x_{1i} - \overline{x_1}) + a_2(x_{2i} - \overline{x_2})\}^2 \\
&= \frac{1}{n} \sum_{i=1}^{n} \{(a_1^2(x_{1i} - \overline{x_1})^2 \\
&\quad + 2a_1 a_2 (x_{1i} - \overline{x_1})(x_{2i} - \overline{x_2}) + (a_2^2(x_{2i} - \overline{x_2})^2\}
\end{aligned}
$$
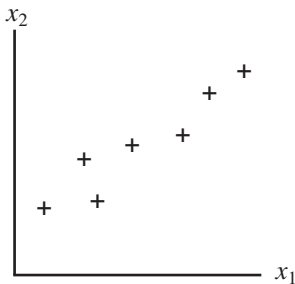
$$
\begin{aligned}
&= a_1^2 \{ \frac{1}{n} \sum_{i=1}^{n} (x_{1i} - \overline{x_1})^2 \} \\
&\quad + 2a_1 a_2 \frac{1}{n} \sum_{i=1}^{n} (x_{1i} - \overline{x_1})(x_{2i} - \overline{x_2}) \\
&\quad + a_2^2 \{ \frac{1}{n} \sum_{i=1}^{n} (x_{2i} - \overline{x_2})^2 \} \\
&= a_1^2 s_{11} + 2a_1 a_2 s_{12} + a_2^2 s_{22} \quad (3)
\end{aligned}
$$

We derive a_1 and a_2 that maximize $V(z_1)$. Assuming that θ_1 and θ_2 are the angles between the vector z_1 and the coordinates x_1 and x_2, respectively, and assuming that

$$ a_1 = \cos \theta_1, \quad a_2 = \cos \theta_2, \quad (4) $$

we get that (a_1, a_2) is the direction cosine of the new coordinate z_1, and a_1 and a_2 satisfy

$$ a_1^2 + a_2^2 = 1. \quad (5) $$

Thus deriving (a_1, a_2) is the maximization of $V(z_1)$ under the condition of Eq. (5).

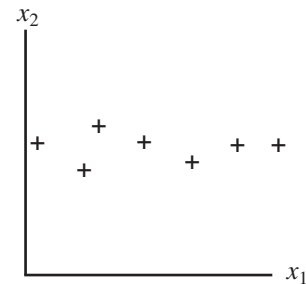Fig. 1: An example of the distribution of two-pixel images (1).

Fig. 2: An example of the distribution of two-pixel images (2).

This kind of conditional maximization problem is solved by Lagrange's method of indeterminate coefficient. By this method, this problem is reduced to the unconditional maximization problem of maximizing

$$ F(a_1, a_2, \lambda) = a_1^2 s_{11} + 2a_1 a_2 s_{12} + a_2^2 s_{22} - \lambda(a_1^2 + a_2^2 - 1), \quad (6) $$

where λ is the indeterminate coefficient. Deriving the partial derivatives of F with respect to a_1, a_2, and λ, and setting them to zero, we get

$$
\begin{aligned}
\frac{\partial F}{\partial a_1} &= 2a_1 s_{11} + 2a_2 s_{12} - 2a_1 \lambda = 0 \\
\frac{\partial F}{\partial a_2} &= 2a_2 s_{22} + 2a_1 s_{12} - 2a_2 \lambda = 0 \\
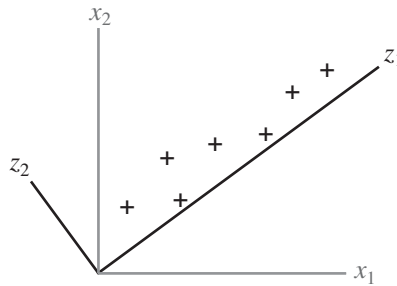\frac{\partial F}{\partial \lambda} &= -\lambda(a_1^2 + a_2^2 - 1) = 0 \quad (7)
\end{aligned}
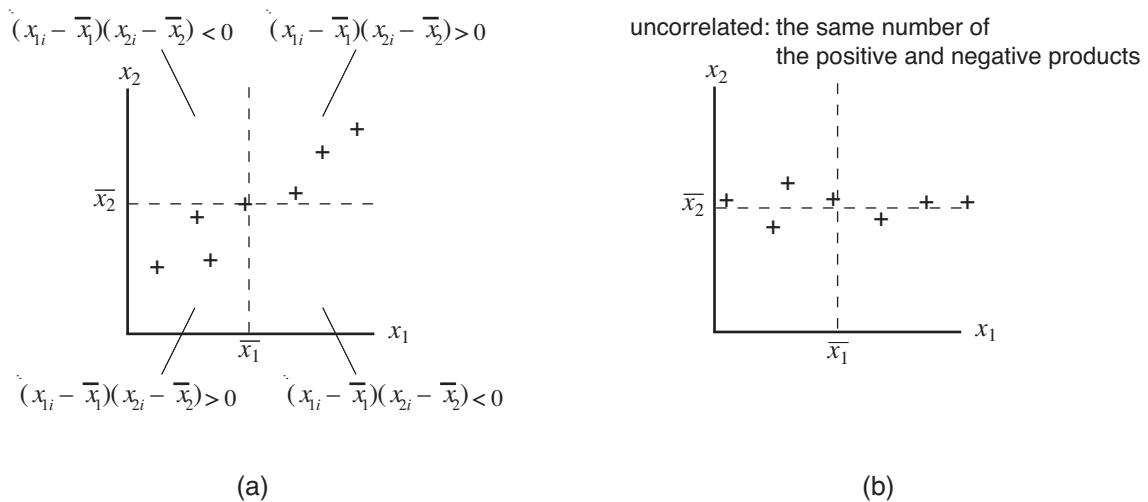$$

Fig. 3: Rotation of the coordinates.

(a)

(b)

Fig. 4: Meaning of covariance. (a) signature of $(x_{1i}-\overline{x_1})(x_{2i}-\overline{x_2})$ in each quadrant. (b) the case of no correlation.

The third equation in Eq. (7) has been already satisfied since it is identical to Eq. (5). From the other two equations, we get

$$
\begin{aligned}
a_1 s_{11} + a_2 s_{12} &= a_1 \lambda \\
a_2 s_{22} + a_1 s_{12} &= a_2 \lambda
\end{aligned} \tag{8}
$$

Rewriting this into the matrix form, we get

$$
\begin{pmatrix} s_{11} & s_{12} \\ s_{12} & s_{22} \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \end{pmatrix} = \lambda \begin{pmatrix} a_1 \\ a_2 \end{pmatrix}. \tag{9}
$$

The matrix in the left side of Eq. (9) is called *covariance matrix*.

Solving Eq. (9) is an eigenvalue problem, where λ is called *eigenvalue* and $\begin{pmatrix} a_1 \\ a_2 \end{pmatrix}$ is called *eigenvector*. The variance $V(z_1)$ is derived as follows: Multiplying

a_1 to the upper equation and a_2 to the lower equation in Eq. (8), we get

$$
\begin{aligned}
a_1^2 s_{11} + a_1 a_2 s_{12} &= \lambda a_1^2 \\
a_1 a_2 s_{12} + a_2^2 s_{22} &= \lambda a_2^2
\end{aligned} \tag{10}
$$

and then

$$
a_1^2 s_{11} + 2a_1 a_2 s_{12} = \lambda(a_1^2 + a_2^2). \tag{11}
$$

From Eq. (3) and Eq. (5), we get

$$
V(z_1) = \lambda. \tag{12}
$$

The eigenvalue problem of Eq. (9) yields two pairs of the eigenvalue λ and the eigenvector as the solutions. Since the problem is the maximization of $V(z_1)$ and the maximum of $V(z_1)$ is equal to λ, the transformed basis z_1 is obtained from the pair with the larger eigenvalue. This basis is called the *first*

principal component, which is "the most important component of image data."

The covariance matrix is symmetric, as shown in Eq. (9), and it is known that the eigenvectors of a symmetric matrix are orthogonal. Thus the other basis z_2 is derived from the other eigenvalue - eigenvector pair yielded as a solution of Eq. (9). The rotation as shown in Fig. 3 is realized by the new coordinates z_1 and z_2. This method is called the *principal component analysis* (PCA).

Principal component analysis and diagonalization

We have considered two-pixel images so far. In this section we extend the method to the case of p-pixel images. In case that the image consists of the pixels $x_1, x_2, \ldots, x_p$, we derive the transformed pixel value

$$z = a_1 x_1 + a_2 x_2 + \cdots + a_p x_p \qquad (13)$$

where the variance of z is maximized subject to $a_1, a_2, \cdots, a_p$. This problem is reduced, similarly to the previous section, to the eigenvalue problem of

$$\begin{pmatrix} s_{11} & s_{12} & \cdots & s_{1p} \\ s_{12} & s_{22} & \cdots & s_{2p} \\ \vdots & & \ddots & \\ s_{p1} & s_{p2} & \cdots & s_{pp} \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \\ \vdots \\ a_p \end{pmatrix} = \lambda \begin{pmatrix} a_1 \\ a_2 \\ \vdots \\ a_p \end{pmatrix}. \qquad (14)$$

where s_{ij} denotes the covariance of x_i and x_j. The p eigenvalues derived from Eq. (14) are, also similarly to the previous section, the variances of p transformed pixel values $z_1, z_2, \ldots, z_p$. Let the eigenvalues be $\lambda_1, \lambda_2, \ldots, \lambda_p$ in descending order, and the corresponding transformed pixel values be $z_1, z_2, \ldots, z_p$, respectively. The pixel value z_1 is "the component of the maximum variance," i. e. "the most important component," and z_2 is the component where the variance is the maximum of the components which are orthogonal to z_1, and so on. The larger the suffix is, the less important the component is. The transformed pixel value z_k is called the *k-th principal component*.

Let $(a_{1(k)}, a_{2(k)}, \ldots, a_{p(k)})'$ be the eigenvector corresponding to the eigenvalue λ_k.[2] From Eq. (13), the

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[2]The symbol $'$ denotes the transposition of a matrix.

k-th principal component z_k is expressed as

$$
\begin{aligned}
z_k &= a_{1(k)} x_1 + a_{2(k)} x_2 + \cdots + a_{p(k)} x_p \\
&= \begin{pmatrix} a_{1(k)} & a_{2(k)} & \cdots & a_{p(k)} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_p \end{pmatrix}. \quad (15)
\end{aligned}
$$

If we denote the covariance matrix in Eq. (14) by S, we get from Eq. (14) as follows:

$$S \begin{pmatrix} a_{1(k)} \\ a_{2(k)} \\ \vdots \\ a_{p(k)} \end{pmatrix} = \lambda_k \begin{pmatrix} a_{1(k)} \\ a_{2(k)} \\ \vdots \\ a_{p(k)} \end{pmatrix} \quad (k = 1, 2, \ldots, p). \quad (16)$$

Combining these equation for $k = 1, 2, \ldots, p$, we get

$$
\begin{aligned}
& S \begin{pmatrix} a_{1(1)} & a_{1(2)} & \cdots & a_{1(p)} \\ a_{2(1)} & a_{2(2)} & \cdots & a_{2(p)} \\ \vdots & & \ddots & \\ a_{p(1)} & a_{p(2)} & \cdots & a_{p(p)} \end{pmatrix} \\
&= \begin{pmatrix} a_{1(1)} & a_{1(2)} & \cdots & a_{1(p)} \\ a_{2(1)} & a_{2(2)} & \cdots & a_{2(p)} \\ \vdots & & \ddots & \\ a_{p(1)} & a_{p(2)} & \cdots & a_{p(p)} \end{pmatrix} \begin{pmatrix} \lambda_1 & & & 0 \\ & \lambda_2 & & \\ & & \ddots & \\ 0 & & & \lambda_p \end{pmatrix}.
\end{aligned}
$$
$$(17)$$

We define a matrix P whose columns are the eigenvectors arranged in descending order of corresponding eigenvalues, i. e.

$$P = \begin{pmatrix} a_{1(1)} & a_{1(2)} & \cdots & a_{1(p)} \\ a_{2(1)} & a_{2(2)} & \cdots & a_{2(p)} \\ \vdots & & \ddots & \\ a_{p(1)} & a_{p(2)} & \cdots & a_{p(p)} \end{pmatrix}, \qquad (18)$$

and define the matrix Λ as follows:

$$\Lambda = \begin{pmatrix} \lambda_1 & & & 0 \\ & \lambda_2 & & \\ & & \ddots & \\ 0 & & & \lambda_p \end{pmatrix}. \qquad (19)$$

Using these expression, we get from Eq. (17) that

$$S P = P \Lambda, \text{ i.e. } P^{-1} S P = \Lambda. \qquad (20)$$

The eigenvectors are normalized, as in Eq. (5) in the case of two-pixel images, and they are orthogonal since S is symmetric, i. e. the eigenvectors form an orthonormal basis. Thus the matrix P is orthonormal. Since $P^{-1} = P'$ if P is orthogonal, we get

$$P'SP = \Lambda, \quad \text{or} \quad S = P\Lambda P'. \qquad (21)$$

The operation is called *diagonalization* of a symmetric matrix S. Since it follows from Eq. (15) for $k = 1, 2, \ldots, p$ that

$$
\begin{pmatrix} z_1 \\ z_2 \\ \vdots \\ z_p \end{pmatrix}
=
\begin{pmatrix}
a_{1(1)} & a_{1(2)} & \cdots & a_{1(p)} \\
a_{2(1)} & a_{2(2)} & \cdots & a_{2(p)} \\
\vdots & & \ddots & \vdots \\
a_{p(1)} & a_{p(2)} & \cdots & a_{p(p)}
\end{pmatrix}
\begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_p \end{pmatrix}
$$

$$
= P' \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_p \end{pmatrix}, \qquad (22)
$$

the matrix P' transforms the original pixel values $x_1, x_2, \ldots, x_p$ to the new pixel values $z_1, z_2, \ldots, z_p$. Such a transformation by an orthogonal matrix is called *orthogonal transformation* of an image. Equation (21 shows that the covariance matrix of the original image set in terms of the pixel values $x_1, x_2, \ldots, x_p$ is obtained by the following operations: "transforming it to the image set in terms of the pixel values $z_1, z_2, \ldots, z_p$ (by P')," "obtaining the diagonal matrix Λ by arranging the eigenvalues," and "inverse-transforming to the image set in terms of the pixel values $x_1, x_2, \ldots, x_p$ (by $(P')^{-1} = P$)." This means that the covariance matrix of the image set by the pixel values $z_1, z_2, \ldots, z_p$ is diagonal and all the covariances are zero, i. e. no pixel values of $z_1, z_2, \ldots, z_p$ correlate to each other.

Karhunen-Loève transformation

The *contribution* of the k-th principal component is defined as the ratio of λ_k to $(\lambda_1 + \lambda_2 + \cdots + \lambda_p)$, i. e. "the ratio of the variance of the k-th principal component to the summation of variances." The contribution indicates "the importance of the transformed pixel," as explained in the first section. Consider the

case that the contributions of the n-th principal components are zero or almost zero for all $n > k$. In the example of the twopixel images in Fig. 2, the contribution of the second principal component is considered almost zero. This means that the variance on the basis corresponding to the second principal component is almost zero, i. e. the variance of the transformed pixel value z_2 is almost zero. It follows that the two-pixel images in terms of pixels x_1 and x_2 can be almost expressed by z_1 only and z_2 of all the images can be replaced with a single value, for example $\overline{z_2}$.

The principal component analysis at first makes the contribution of the first principal component as large as possible, and then the contribution of the second one as large as possible, and so on. In other words, the principal component analysis makes the contribution of the last principal components as small as possible. It means that omitting the several last principal components yields the smallest errors in the cases that a certain number of pixels are omitted. The principal component analysis has an ability of reducing the data amount while the information of the original data is preserved as much as possible.

If we consider the case that there are many p-pixel images, and assume that only $p/2$ pixels are available for one communication channel at a time. How can we transmit the images while the information of the original image is preserved as much as possible? As shown so far, the answer is as follows: the image is transformed to the principal components and only the top $p/2$ principal components are transmitted. In this sense, the orthogonal transformation of Eq. (22) is called *Karhunen-Loève transformation*.

The receiver calculates the inverse transformation, i. e. transformation from z to x, to obtain the images which are almost the same as the original ones. This

inverse transformation is as follows:

$$\begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_p \end{pmatrix} \simeq (P')^{-1} \begin{pmatrix} z_1 \\ z_2 \\ \vdots \\ z_{p/2} \\ \overline{z_{p/2+1}} \\ \vdots \\ \overline{z_p} \end{pmatrix} = P \begin{pmatrix} z_1 \\ z_2 \\ \vdots \\ z_{p/2} \\ \overline{z_{p/2+1}} \\ \vdots \\ \overline{z_p} \end{pmatrix}. \quad (23)$$

This method requires the covariance matrix of all the images; it is generally impossible. If we assume the ergodicity[3], which is the property that the covari- ances among the images can be replaced with the co- variances within an image, of the images under con- sideration, the covariance matrix can be calculated from one image; This property, however, does not hold for practical images generally.

To avoid this problem, it is widely applied to choose a fixed set of basis vectors instead of calculat- ing the principal components. The data compression error of this basis is not the smallest, but sufficiently small for almost all practical images. It will be ex- plained in the following two sessions how to choose an appropriate basis.
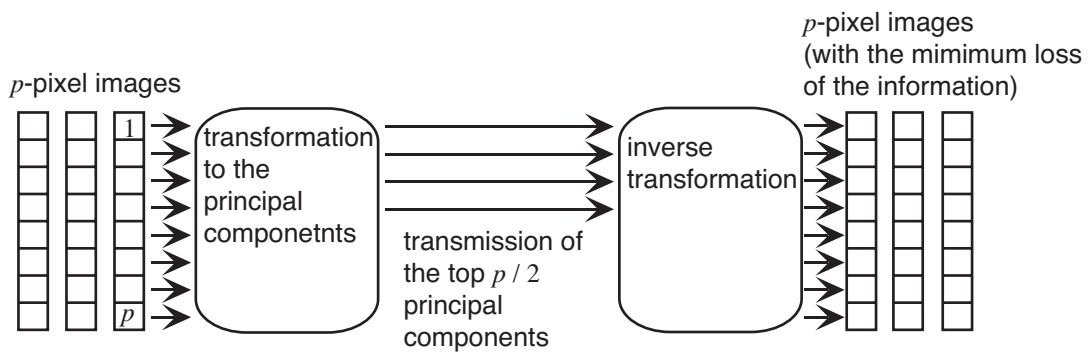

Fig. 5: Image compression by the KL transformation.

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[3]See the references presented at the beginning of this course, for example: M. Petrou and P. Bosdogianni, *Image Processing The Fundamentals,* for details.