Decorrelation in Statistics: The Mahalanobis Transformation

Added material to *Data Compression: The Complete Reference*

An image can be compressed if, and only if, its pixels are correlated. This is mentioned many times in Chapter 4, as well as the fact that any image compression method results in *decorrelating* the pixels. As a result, any transformation that decorrelates values can be the basis for an image compression method. Several such transformations are described in Section 4.4.

The topic of this document is the little-known *Mahalanobis transformation*, used by statisticians to decorrelate two random variables. The discussion starts by defining the square root of a matrix and the concept of a centring matrix. This is followed by a review of the concepts of mean, variance, and covariance, in order to derive relations that are needed later. The transformation and its inverse are then introduced and *Mathematica* and Matlab codes for it are provided. A proof is included, to show that this transformation really decorrelates the two variables.

Matrix Concepts. This short section shows (1) how a matrix A can be raised to any rational power r/s and (2) the definition of the centring matrix H.

The spectral decomposition (also known as the Jordan decomposition) theorem claims that any symmetric matrix A can be written as

$$A = \Gamma\Lambda\Gamma^T,$$

Where Λ is a diagonal matrix of the eigenvalues λ_i of A and Γ is an orthogonal matrix whose columns are the standardized eigenvectors of A.

A corollary of this theorem is that if A is a nonsingular symmetric matrix, then for any integer n

$$\Lambda^n = \text{diag}(\lambda_i^n) \quad \text{and} \quad A^n = \Gamma\Lambda^n\Gamma^T.$$

In addition, if all the eigenvalues of A are positive, then any rational power $A^{r/s}$ of A (for integers $s > 0$ and r) can be defined as

$$A^{r/s} = \Gamma\Lambda^{r/s}\Gamma^T, \quad \text{where} \quad \Lambda^{r/s} = \text{diag}(\lambda_i^{r/s}).$$

Two important special cases of this corollary are (we use the notation X' for a transpose)

$$A^{1/2} = \Gamma\Lambda^{1/2}\Gamma', \quad \text{where} \quad \Lambda^{1/2} = \text{diag}(\sqrt{\lambda_i}), \tag{1}$$

(this is the symmetric square root decomposition of A; it exists when $\lambda_i \ge 0$) and

$$A^{-1/2} = \Gamma\Lambda^{-1/2}\Gamma', \quad \text{where} \quad \Lambda^{-1/2} = \text{diag}(1/\sqrt{\lambda_i}), \tag{2}$$

(this matrix exists when $\lambda_i > 0$). Direct multiplication verifies that $A^{1/2}A^{1/2} = A$ and $A^{1/2}A^{-1/2} = I$.

The *centring* matrix H is defined as

$$\mathbf{H} = \mathbf{I} - \frac{1}{n}\mathbf{J}, \tag{3}$$

where $\mathbf{I}$ is the identity matrix and $\mathbf{J}$ is a matrix of all 1's. Direct multiplication verifies that $\mathbf{H}$ is symmetric $\mathbf{H} = \mathbf{H}'$ and idempotent $\mathbf{H^2} = \mathbf{H}$.

Basic Statistical Concepts

The correlations discussed here are between *random variables*. The dictionary definition of this term is "a variable whose values are random but whose statistical distribution is known."

Given a set of n random variables with p values each, we write them as the rows of a data matrix $\mathbf{A}_{np}$. As an example consider the heights, weights, and incomes of p persons. There are p values for each of the 3 variables, so matrix $\mathbf{A}$ has three rows and p columns. We don't expect the columns to show any correlation, but the rows may be correlated. It is known from experience that there is a strong correlation between the height and weight of a person, but weak or no correlation between height and income.

We denote the elements of $\mathbf{A}$ by a_{ij} where $i = 1, 2, \ldots, n$ and $j = 1, 2, \ldots, p$. Row i of $\mathbf{A}$ is denoted by $\mathbf{a}_{i*}$ and column j is denoted by $\mathbf{a}_{*j}$. The notation $\mathbf{a}'_{i*}$ refers to row i written vertically, as a column (i.e., transposed).

The *mean* of random variable j (i.e., column j of $\mathbf{A}$) is denoted by $\bar{a}_j$ and is given by the familiar expression

$$\bar{a}_j = \frac{1}{n}\sum_{k=1}^{n} a_{kj} = \frac{1}{n}\mathbf{a}_{*j}, \quad j = 1, 2, \ldots, p.$$

We arrange the individual means $\bar{a}_j$ in the *mean vector* $\bar{\mathbf{a}}$

$$\bar{\mathbf{a}} = \begin{pmatrix} \bar{a}_1 \\ \bar{a}_2 \\ \vdots \\ \bar{a}_p \end{pmatrix} = \frac{1}{n}\left[\begin{pmatrix} a_{11} \\ a_{21} \\ \vdots \\ a_{n1} \end{pmatrix} + \begin{pmatrix} a_{12} \\ a_{22} \\ \vdots \\ a_{n2} \end{pmatrix} + \cdots + \begin{pmatrix} a_{1p} \\ a_{2p} \\ \vdots \\ a_{np} \end{pmatrix}\right] = \frac{1}{n}\sum_{k=1}^{n} \mathbf{a}'_{k*} = \mathbf{A}' \cdot \mathbf{1}, \quad (4)$$

where $\mathbf{1}$ denotes a column of n 1's.

The *variance* of the same variable is defined as

$$s_{jj} = \frac{1}{n}\sum_{k=1}^{n}(a_{kj} - \bar{a}_j)^2, \quad j = 1, 2, \ldots, p. \quad (5)$$

If all the values a_{kj} are close to the mean $\bar{a}_j$, the variance is small, indicating that the variable does not vary much.

From the definition of the variance, we get a natural definition for the *covariance* of variables i and j

$$s_{ij} = \frac{1}{n}\sum_{k=1}^{n}(a_{ki} - \bar{a}_i)(a_{kj} - \bar{a}_j), \quad i, j = 1, 2, \ldots, p.$$

The covariance measures the association between the variables. If the two differences $a_{ki} - \bar{a}_i$ and $a_{kj} - \bar{a}_j$ have the same sign (i.e., if both values a_{ki} and a_{kj} are above or both are below their averages), then the term $(a_{ki}-\bar{a}_i)(a_{kj}-\bar{a}_j)$ is positive and contributes toward increasing the covariance. If the two differences have opposite signs, then their product is negative and it decreases the covariance. The covariance of two variables is the basis for the definition of the *correlation coefficient* of the variables.

The *standard deviation* is also an important statistical measure. It is defined as the square root of the variance.

We denote by $\mathbf{S}_A$ the $p\times p$ matrix whose elements are the covariances s_{ij} of the columns of $\mathbf{A}$. Equation (5) implies that

$$\mathbf{S}_A=\frac{1}{n}\sum_{k=1}^{n}(\mathbf{a}_{k*}-\bar{\mathbf{a}})(\mathbf{a}_{k*}-\bar{\mathbf{a}})'=\frac{1}{n}\sum_{k=1}^{n}\mathbf{a}_{k*}\mathbf{a}'_{k*}-\bar{\mathbf{a}}\,\bar{\mathbf{a}}'.$$

This can also be written

$$\mathbf{S}_A=\frac{1}{n}\mathbf{A}'\mathbf{A}-\bar{\mathbf{a}}\,\bar{\mathbf{a}}'=\frac{1}{n}\left(\mathbf{A}'\mathbf{A}-\frac{1}{n}\mathbf{A}'\mathbf{J}\mathbf{A}\right),$$

where $\mathbf{J}$ is a matrix of all 1's. Using Equation (4) and the centring matrix $\mathbf{H}$ [Equation (3)], we end up with the following compact expression for the covariance matrix

$$\mathbf{S}_A=\frac{1}{n}\mathbf{A}'\mathbf{H}\mathbf{A}. \tag{6}$$

It can be shown that the eigenvalues of the covariance matrix $\mathbf{S}_A$ are nonnegative, so $\mathbf{S}_A$ is a *positive semi-definite* matrix. In addition, if $n\geq p+1$, then the eigenvalues of $\mathbf{S}_A$ are normally all positive, and $\mathbf{S}_A$ is a *positive definite* matrix.

The covariance s_{ij} expresses the amount of correlation between variables i and j. Large positive values of s_{ij} mean strong positive correlation. Small values mean no correlation, and negative values imply negative correlation. The Pearson correlation coefficient R_{ij} discussed later is based on s_{ij}.

The Transformation

The Mahalanobis decorrelation transformation is applied to the n rows of $\mathbf{A}$. Each row $\mathbf{a}_{k*}$ is transformed to the row

$$\mathbf{z}_{k*}=\mathbf{S}_A^{-1/2}(\mathbf{a}_{k*}-\bar{\mathbf{a}}),\quad \text{for}\quad k=1,2,\ldots,n, \tag{7}$$

where $\mathbf{S}_A^{-1/2}$ is given by Equation (2). If $\mathbf{S}_A$ is positive definite, then $\mathbf{S}_A^{-1/2}$ is symmetric positive definite. The proof below shows that the covariance matrix $\mathbf{S}_Z$ of the n vectors $\mathbf{Z}=(\mathbf{z}_{1*},\mathbf{z}_{2*},\ldots,\mathbf{z}_{n*})$ is the identity matrix, implying that these vectors are decorrelated. Figure 1a is simple *Mathematica* code to calculate this transformation. Figure 1b, adapted from [Mahab 00], is Matlab code for the same task.

An important point is that the transformation is reversible. This is since [from Equations (1–2)] $\mathbf{S}_A^{-1/2}$ is the inverse of $\mathbf{S}_A^{1/2}$. Equation (7) implies that the rows

```
Needs["Statistics`MultiDescriptiveStatistics`"]
Clear[A,Z,S,S5,d1,d2];
A={{1,2,3},{2.1,4,6.5},{3,7,9},{4.4,8.2,12}};
 (* Test data. The columns of A are correlated *)
S=CovarianceMatrix[A];
Llamda=DiagonalMatrix[1/Sqrt[Eigenvalues[S]]];
Ggama=Transpose[Eigenvectors[S]];
 (* Eigenvectors are the COLUMNS of Ggama *)
S5=Ggama.Llamda.Transpose[Ggama]; (* S^{-1/2} *)
S-Inverse[S5.S5]; (* Test. Should be all zeros *)
{d1,d2}=Dimensions[A]; (* # of rows & columns of A *)
Z=Array[0,{d1,d2}]; (* Construct null matrix Z *)
Do[Z[[i]]=S5.(A[[i]]-Mean[A]), {i,d1}]
 (* Construct d1 rows of Z *)
Mean[Z] (* All zeros *)
Variance[Z] (* All 1's, so Z is standardized *)
CovarianceMatrix[Z] (* The identity matrix,
                       so Z is decorrelated! *)
```

Figure 1. (a) Mathematica code for the Mahalanobis Transformation

```
clear
x=[1 2 3 4; 4 3 2 2; 4 6 7 5; 9 8 2 1];
s=cov(x);                     % empirical covariance
[eigvec,eigval]=eig(s);       % spectral decomposition
eigval=diag(eigval);
tmp=sort([eigval,eigvec],1);
% sort by eigenvalues (col. 1) ascending
tmp=flipud(tmp);              % Flip to get descending sort
eigval=tmp(:,1);
[r,c]=size(tmp);
eigvec=tmp(:,2:c)';
eigval                       % eigenvalues
eigvec                       % eigenvectors
sqrt(eigval)
eigval1=1./sqrt(eigval)      % computes lambda to the power -1/2
eigval1=diag(eigval1)        % makes diagonal matrix from lambda2
s2=eigvec*eigval1*eigvec'    % computes s to the power -1/2
x=x-mean(x)                  % corrects for mean
z=x*s2                       % Mahalanobis transformation
mean(z)                      % show mean of z
cov(z)                       % show empirical covariance of z
```

Figure 1. (b) Matlab code for the Mahalanobis Transformation

of **A** can be reconstructed by

$$\mathbf{a}_{k*} = \mathbf{S}_A^{1/2}\mathbf{z}_{k*} + \bar{\mathbf{a}}, \quad \text{for} \quad k = 1, 2, \ldots, n.$$

Proof of Decorrelation

Step 1. From the definition of **Z** [Equation (7)] and from the fact that $\mathbf{S}_A^{-1/2}$ is symmetric (and thus equals its transpose) we get

$$\mathbf{Z} = \mathbf{H}\cdot\mathbf{A}\cdot\mathbf{S}_A^{-1/2},$$

where **H** is the centring matrix [Equation (3)].

Step 2. We apply the properties of the centring **H** to show

$$\begin{aligned}
\mathbf{S}_Z &\overset{*}{=} \frac{1}{n}\mathbf{Z}'\mathbf{H}\mathbf{Z} \\
&= \frac{1}{n}(\mathbf{S}_A^{-1/2}\,\mathbf{A}'\mathbf{H}')\mathbf{H}(\mathbf{H}\,\mathbf{A}\,\mathbf{S}_A^{-1/2}) \\
&= \mathbf{S}_A^{-1/2}(\frac{1}{n}\mathbf{A}'\mathbf{H}\mathbf{A})\mathbf{S}_A^{-1/2} \\
&\overset{*}{=} \mathbf{S}_A^{-1/2}\mathbf{S}_A\mathbf{S}_A^{-1/2} = \mathbf{S}_A^{1/2}\mathbf{S}_A^{-1/2} = \mathbf{I}.
\end{aligned}$$

[The two equalities marked with "$*$" employ Equation (6).] End of proof.

> The Academy admits, then, that divinity and humanity are identical, or at least correlative; but the question now is in what consists this correlation: such is the meaning of the problem of certainty, such is the object of social philosophy.
>
> Joseph-Pierre Proudhon *The Philosophy of Misery*

References

Mahab 2000 is URL `http://www.quantlet.de/codes/sma/mahabank_right.html`.

Mardia, K. V., J. T. Kent, and J. M. Bibby, *Multivariate Analysis*, Academic Press, 1979.

Rudra, Ashok, *Prasanta Chandra Mahalanobis: A Biography*, Oxford University Press, New Delhi, 1996.

December 7, 2000

Prasanta Chandra Mahalanobis [1893–1972]

One of the greatest scientists of 20th century India, P. C. Mahalanobis has been described as a "renaissance man and scientist." Born in 1893, he graduated with honors in Physics from Presidency College, Calcutta in 1912. He went to England in 1915 and completed the Tripos in Mathematics and Physics from King's College, Cambridge. He then left England and spent his entire career in Calcutta. He became interested in statistics, and personally established the widespread use of this science in India.

His greatest scientific achievement was (in 1927) the D^2 statistic, that became known as the "Mahalanobis Distance." He was also an administrator and his greatest achievement in this field was the establishment, in 1931, of the Indian Statistical Institute (ISI), one of the best centers for statistical research and practical work in the world. He had close relationships with important statisticians such as R. A. Fisher and Karl Pearson, and managed to attract many world-class scientists to the institute. The "professor,"—as he was referred to by everyone in the Institute,—and his wife, Nirmal Kumari, poured in all they possessed to establish the Institute on a firm footing. In 1959, the Institute was declared an "Institution of National Importance" by an act of the Indian Parliament.

In 1957, Mahalanobis became the Honorary President of the International Statistical Institute, and was elected a fellow of the American Statistical Association in 1961. Throughout his career he received many other academic honors and awards. He received the highest national honor, Padma Vibhushan, from the President of India in 1968.

[Rudra 96] is a biography of P. C. Mahalanobis.