Principal component analysis

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Introduction

Supervised learning: prediction of y from $x_1, \ldots, x_p$

Multiple regression (interval response): $y = f(x_1, \ldots, x_p) + \varepsilon$

Binary logistic regression: $\pi = \dfrac{\exp\{f(x_1, \ldots, x_p)\}}{1 + \exp\{f(x_1, \ldots, x_p)\}}$

If p is large compared to N, then the problem of overfitting might arise

Solutions to overfitting

- More data
- Regularization (Ridge regression and Lasso)
- Principal components regression

Introduction

The $N \times p$ data matrix

$$\mathbf{X} = \begin{bmatrix} x_{11} & x_{12} & \dots & x_{1p} \\ x_{21} & x_{22} & \dots & x_{2p} \\ \vdots & \vdots & & \vdots \\ x_{N1} & x_{N2} & \dots & x_{Np} \end{bmatrix}$$

Example 1: 9×2 data matrix

$$\mathbf{X} = \begin{bmatrix} 7.73 & 11.86 \\ 7.73 & 19.19 \\ 1.91 & 4.53 \\ 4.82 & 11.86 \\ 10.65 & 19.19 \\ 10.65 & 26.52 \\ 16.48 & 33.85 \\ 13.56 & 19.19 \\ 16.48 & 33.85 \end{bmatrix}$$

Introduction

The transpose of the data matrix

$$\mathbf{X}^T = \begin{bmatrix} x_{11} & x_{21} & \dots & x_{N1} \\ x_{12} & x_{22} & \dots & x_{N2} \\ \vdots & \vdots & & \vdots \\ x_{1p} & x_{2p} & \dots & x_{Np} \end{bmatrix}$$

Example 1 (continued)

$$\mathbf{X}^T = \begin{bmatrix} 7.73 & 7.73 & 1.91 & 4.82 & 10.65 & 10.65 & 16.48 & 13.56 & 16.48 \\ 11.86 & 19.19 & 4.53 & 11.86 & 19.19 & 26.52 & 33.85 & 19.19 & 33.85 \end{bmatrix}$$

Introduction

The data vector of feature j is

$$\mathbf{x}_j = \begin{bmatrix} x_{1j} \\ x_{2j} \\ \vdots \\ x_{Nj} \end{bmatrix}$$

The data vector of case i is

$$x_i = [\, x_{i1} \; x_{i2} \; \ldots \; x_{ip} \,]^T$$

So the data matrix equals

$$\mathbf{X} = [\, \mathbf{x}_1 \; \mathbf{x}_2 \; \ldots \; \mathbf{x}_p \,] = [\, x_1 \; x_2 \; \ldots \; x_N \,]^T$$

Introduction

The mean of feature j is

$$\bar{x}_j = \sum_{i=1}^{N} x_{ij}/N$$

The mean vector is

$$\bar{x} = \left[\, \bar{x}_1 \;\; \ldots \;\; \bar{x}_p \,\right]^T$$

Example 1 (continued)

$$\bar{x} = \left[\, 10 \;\; 20 \,\right]^T$$

Introduction

The centered data vector of case i is

$$\tilde{x}_i = [\,\tilde{x}_{i1}\ \ldots\ \tilde{x}_{ip}\,]^T = x_i - \bar{x} = [\,x_{i1} - \bar{x}_1\ \ldots\ x_{ip} - \bar{x}_p\,]^T$$

The centered data matrix is

$$\tilde{\mathbf{X}} = [\,\tilde{x}_1\ \tilde{x}_2\ \ldots\ \tilde{x}_N\,]^T = [\,\tilde{\mathbf{x}}_1\ \tilde{\mathbf{x}}_2\ \ldots\ \tilde{\mathbf{x}}_p\,]$$

Example 1 (continued)

$$\tilde{\mathbf{X}} = \begin{bmatrix} 7.73 - 10 & 11.86 - 20 \\ 7.73 - 10 & 19.19 - 20 \\ 1.91 - 10 & 4.53 - 20 \\ 4.82 - 10 & 11.86 - 20 \\ 10.65 - 10 & 19.19 - 20 \\ 10.65 - 10 & 26.52 - 20 \\ 16.48 - 10 & 33.85 - 20 \\ 13.56 - 10 & 19.19 - 20 \\ 16.48 - 10 & 33.85 - 20 \end{bmatrix} = \begin{bmatrix} -2.27 & -8.14 \\ -2.27 & -0.81 \\ -8.09 & -15.47 \\ -5.18 & -8.14 \\ 0.65 & -0.81 \\ 0.65 & 6.52 \\ 6.48 & 13.85 \\ 3.56 & -0.81 \\ 6.48 & 13.85 \end{bmatrix}$$

Introduction

The sample covariance between features j and k is

$$s_{jk} = \tilde{\mathbf{x}}_j^T \tilde{\mathbf{x}}_k / N = \sum_{i=1}^{N} \tilde{x}_{ij} \tilde{x}_{ik} / N = (\tilde{x}_{1j} \tilde{x}_{1k} + \ldots + \tilde{x}_{Nj} \tilde{x}_{Nk}) / N$$

where $\tilde{\mathbf{x}}_j^T \tilde{\mathbf{x}}_k$ is called the dot product of vectors $\tilde{\mathbf{x}}_j$ and $\tilde{\mathbf{x}}_k$

The sample variance of feature j is $s_{jj} = \tilde{\mathbf{x}}_j^T \tilde{\mathbf{x}}_j / N = s_j^2$

The sample covariance matrix is the symmetric matrix

$$\mathbf{S} = \begin{bmatrix} s_1^2 & & & \\ s_{21} & s_2^2 & & \\ \vdots & \vdots & \ddots & \\ s_{p1} & s_{p2} & \ldots & s_p^2 \end{bmatrix} = \mathbf{S}^T$$

Introduction

The sample covariance matrix equals

$$\mathbf{S} = \tilde{\mathbf{X}}^T\tilde{\mathbf{X}}/N = \frac{1}{N}\begin{bmatrix} \tilde{\mathbf{x}}_1^T\tilde{\mathbf{x}}_1 & & & \\ \tilde{\mathbf{x}}_2^T\tilde{\mathbf{x}}_1 & \tilde{\mathbf{x}}_2^T\tilde{\mathbf{x}}_2 & & \\ \vdots & \vdots & \ddots & \\ \tilde{\mathbf{x}}_p^T\tilde{\mathbf{x}}_1 & \tilde{\mathbf{x}}_p^T\tilde{\mathbf{x}}_2 & \dots & \tilde{\mathbf{x}}_p^T\tilde{\mathbf{x}}_p \end{bmatrix}$$

The total variance is defined as the trace of $\mathbf{S}$ given by

$$\text{tr}(\mathbf{S}) = \sum_{j=1}^{p} s_j^2 = s_1^2 + s_2^2 + \ldots + s_p^2 = \frac{1}{N}\sum_{j=1}^{p}\tilde{\mathbf{x}}_j^T\tilde{\mathbf{x}}_j$$

Research question: Can most of the total variance be explained by a smaller than p number of dimensions?

Principal components

Principal components are weighted sums of the centered features

The principal component scores

$$\hat{\mathbf{\Lambda}} = \begin{bmatrix} \hat{\lambda}_{11} & \hat{\lambda}_{12} & \dots & \hat{\lambda}_{1p} \\ \hat{\lambda}_{21} & \hat{\lambda}_{22} & \dots & \hat{\lambda}_{2p} \\ \vdots & \vdots & & \vdots \\ \hat{\lambda}_{N1} & \hat{\lambda}_{N2} & \dots & \hat{\lambda}_{Np} \end{bmatrix} = \tilde{\mathbf{X}}\mathbf{V} = \begin{bmatrix} \tilde{x}_1^T\mathbf{v}_1 & \tilde{x}_1^T\mathbf{v}_2 & \dots & \tilde{x}_1^T\mathbf{v}_p \\ \tilde{x}_2^T\mathbf{v}_1 & \tilde{x}_2^T\mathbf{v}_2 & \dots & \tilde{x}_2^T\mathbf{v}_p \\ \vdots & \vdots & & \vdots \\ \tilde{x}_N^T\mathbf{v}_1 & \tilde{x}_N^T\mathbf{v}_2 & \dots & \tilde{x}_N^T\mathbf{v}_p \end{bmatrix}$$

where the columns of $\mathbf{V} = [\,\mathbf{v}_1 \;\mathbf{v}_2 \;\dots\; \mathbf{v}_p\,]$ are the vectors of weights

The score of case i on principal component j is

$$\hat{\lambda}_{ij} = \tilde{x}_i^T\mathbf{v}_j = v_{1j}\tilde{x}_{i1} + v_{2j}\tilde{x}_{i2} + \dots + v_{kj}\tilde{x}_{ip}$$

Principal components

How are $\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_p$ (columns of weights) chosen?

Since the mean of the scores on the first principal component is zero, the variance equals

$$\frac{1}{N}\sum_{i=1}^{N}\hat{\lambda}_{i1}^2 = \frac{1}{N}\sum_{i=1}^{N}(\tilde{x}_i^T\mathbf{v}_1)^2$$

The elements of $\mathbf{v}_1$ are chosen such that this variance is maximum, subject to the constraint that $\mathbf{v}_1^T\mathbf{v}_1 = 1$

Principal components

Since the mean of the scores on the second principal component is zero, the variance equals

$$\frac{1}{N}\sum_{i=1}^{N}\hat{\lambda}_{i2}^{2} = \frac{1}{N}\sum_{i=1}^{N}(\tilde{x}_i^T\mathbf{v}_2)^2$$

The elements of $\mathbf{v}_2$ are chosen such that this variance is maximum, subject to the constraints that $\mathbf{v}_2^T\mathbf{v}_2 = 1$ and $\mathbf{v}_1^T\mathbf{v}_2 = 0$

Principal components

Since the mean of the scores on the third principal component is zero, the variance equals

$$\frac{1}{N}\sum_{i=1}^{N}\hat{\lambda}_{i3}^2 = \frac{1}{N}\sum_{i=1}^{N}(\tilde{x}_i^T\mathbf{v}_3)^2$$

The elements of $\mathbf{v}_3$ are chosen such that this variance is maximum, subject to the constraints that $\mathbf{v}_3^T\mathbf{v}_3 = 1$, $\mathbf{v}_1^T\mathbf{v}_3 = 0$, and $\mathbf{v}_2^T\mathbf{v}_3 = 0$

And so on up to the pth principal component

Singular value decomposition

The matrix of centered data can be decomposed as

$$\tilde{\mathbf{X}} = \mathbf{U}\mathbf{D}\mathbf{V}^T$$

where

- $\mathbf{U} = [\, \mathbf{u}_1 \ \ldots \ \mathbf{u}_p \,]$ is an $N \times p$ semi-orthogonal matrix whose columns are called the left singular vectors
- $\mathbf{V} = [\, \mathbf{v}_1 \ \ldots \ \mathbf{v}_p \,]$ is an $p \times p$ orthogonal matrix whose columns are called the right singular vectors
- $\mathbf{D}$ is a $p \times p$ diagonal matrix with diagonal elements $d_1 \geq d_2 \geq \ldots \geq d_p \geq 0$ known as the singular values

Singular value decomposition

$\mathbf{U}$ is a semi-orthogonal matrix, that is,

$$\mathbf{U}^T\mathbf{U} = \begin{bmatrix} \mathbf{u}_1^T\mathbf{u}_1 & \mathbf{u}_1^T\mathbf{u}_2 & \dots & \mathbf{u}_1^T\mathbf{u}_p \\ \mathbf{u}_2^T\mathbf{u}_1 & \mathbf{u}_2^T\mathbf{u}_2 & \dots & \mathbf{u}_2^T\mathbf{u}_p \\ \vdots & \vdots & & \vdots \\ \mathbf{u}_p^T\mathbf{u}_1 & \mathbf{u}_p^T\mathbf{u}_2 & \dots & \mathbf{u}_p^T\mathbf{u}_p \end{bmatrix} = \begin{bmatrix} 1 & 0 & \dots & 0 \\ 0 & 1 & \dots & 0 \\ \vdots & \vdots & & \vdots \\ 0 & 0 & \dots & 1 \end{bmatrix} = \mathbf{I}$$

where $\mathbf{I}$ is called the identity matrix

$\mathbf{V}$ is an orthogonal matrix, that is, $\mathbf{V}^T\mathbf{V} = \mathbf{I} = \mathbf{V}\mathbf{V}^T$

Singular value decomposition

D is a diagonal matrix, that is,

$$\mathbf{D} = \begin{bmatrix} d_1 & 0 & \dots & 0 \\ 0 & d_2 & \dots & 0 \\ \vdots & \vdots & & \vdots \\ 0 & 0 & \dots & d_p \end{bmatrix}$$

where $d_1 \geq d_2 \geq \dots \geq d_p \geq 0$

Singular value decomposition

Example 1 (continued)

$$\tilde{\mathbf{X}} = \begin{bmatrix} -2.27 & -8.14 \\ -2.27 & -0.81 \\ -8.09 & -15.47 \\ -5.18 & -8.14 \\ 0.65 & -0.81 \\ 0.65 & 6.52 \\ 6.48 & 13.85 \\ 3.56 & -0.81 \\ 6.48 & 13.85 \end{bmatrix} = \underbrace{\begin{bmatrix} -0.27 & -0.29 \\ -0.05 & 0.34 \\ -0.56 & 0.13 \\ -0.31 & 0.24 \\ -0.01 & -0.19 \\ 0.20 & 0.44 \\ 0.49 & 0.02 \\ 0.03 & -0.71 \\ 0.49 & 0.02 \end{bmatrix}}_{\mathbf{U}} \underbrace{\begin{bmatrix} 31.22 & 0.00 \\ 0.00 & 5.03 \end{bmatrix}}_{\mathbf{D}} \underbrace{\begin{bmatrix} 0.43 & 0.90 \\ -0.90 & 0.43 \end{bmatrix}}_{\mathbf{V}^T}$$

Singular value decomposition

The $N \times p$ matrix of principal component scores can be calculated through

$$\hat{\mathbf{\Lambda}} = \begin{bmatrix} \hat{\lambda}_{11} & \ldots & \hat{\lambda}_{1p} \\ \vdots & & \vdots \\ \hat{\lambda}_{N1} & \ldots & \hat{\lambda}_{Np} \end{bmatrix} = \tilde{\mathbf{X}}\mathbf{V} = \mathbf{U}\mathbf{D}$$

The score of case i on principal component j is

$$\hat{\lambda}_{ij} = v_{1j}\tilde{x}_{i1} + v_{2j}\tilde{x}_{i2} + \ldots + v_{pj}\tilde{x}_{ip} = \mathbf{v}_j^T\tilde{x}_i = u_{ij}d_j$$

The variance of the jth principal component is

$$\frac{1}{N}\sum_{i=1}^{N}\hat{\lambda}_{ij}^2 = \frac{1}{N}\sum_{i=1}^{N}(u_{ij}d_j)^2 = \frac{d_j^2}{N}\sum_{i=1}^{N}u_{ij}^2 = \frac{d_j^2}{N}\mathbf{u}_j^T\mathbf{u}_j = \frac{d_j^2}{N}$$

Principal components

Example 1 (continued)

$$\hat{\mathbf{\Lambda}} = \underbrace{\begin{bmatrix} -2.27 & -8.14 \\ -2.27 & -0.81 \\ -8.09 & -15.47 \\ -5.18 & -8.14 \\ 0.65 & -0.81 \\ 0.65 & 6.52 \\ 6.48 & 13.85 \\ 3.56 & -0.81 \\ 6.48 & 13.85 \end{bmatrix} \begin{bmatrix} 0.43 & -0.90 \\ 0.90 & 0.43 \end{bmatrix}}_{\tilde{\mathbf{X}}\mathbf{V}} = \begin{bmatrix} -8.33 & -1.45 \\ -1.71 & 1.70 \\ -17.45 & 0.67 \\ -9.58 & 1.19 \\ -0.46 & -0.93 \\ 6.16 & 2.21 \\ 15.28 & 0.09 \\ 0.79 & -3.57 \\ 15.28 & 0.09 \end{bmatrix}$$

Principal components

Example 1 (continued)

$$\hat{\mathbf{\Lambda}} = \underbrace{\begin{bmatrix} -0.27 & -0.29 \\ -0.05 & 0.34 \\ -0.56 & 0.13 \\ -0.31 & 0.24 \\ -0.01 & -0.19 \\ 0.20 & 0.44 \\ 0.49 & 0.02 \\ 0.03 & -0.71 \\ 0.49 & 0.02 \end{bmatrix} \begin{bmatrix} 31.22 & 0.00 \\ 0.00 & 5.03 \end{bmatrix}}_{\mathbf{UD}} = \begin{bmatrix} -8.33 & -1.45 \\ -1.71 & 1.70 \\ -17.45 & 0.67 \\ -9.58 & 1.19 \\ -0.46 & -0.93 \\ 6.16 & 2.21 \\ 15.28 & 0.09 \\ 0.79 & -3.57 \\ 15.28 & 0.09 \end{bmatrix}$$

Principal components

Example 1 (continued)

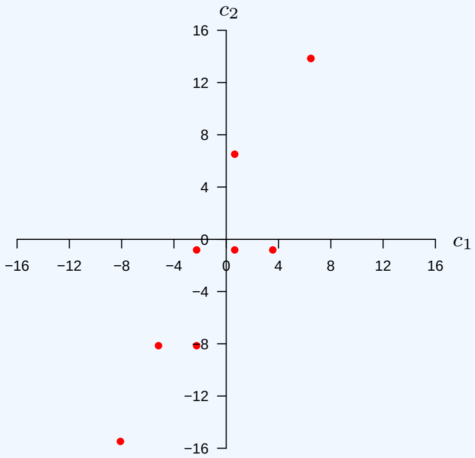
Two centered features

	i	$\tilde{x}_{i1}$	$\tilde{x}_{i2}$
	1	-2.27	-8.14
	2	-2.27	-0.81
	3	-8.09	-15.47
	4	-5.18	-8.14
case	5	0.65	-0.81
	6	0.65	6.52
	7	6.48	13.85
	8	3.56	-0.81
	9	6.48	13.85

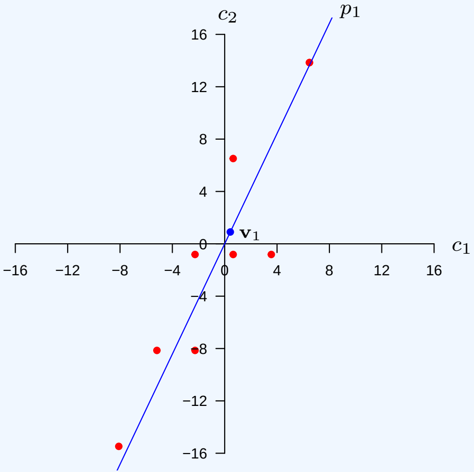
In the case of 2 features, 2 principal components are constructed

$$\hat{\lambda}_{i1} = \mathbf{v}_1^T \tilde{x}_i$$
$$\hat{\lambda}_{i2} = \mathbf{v}_2^T \tilde{x}_i$$

Example 1 (continued)



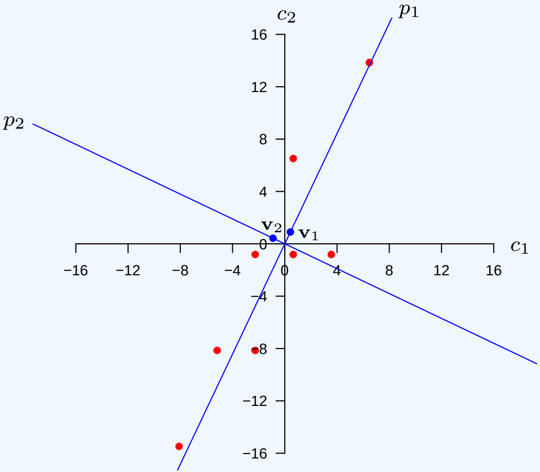
Example 1 (continued)



$\mathbf{v}_1 = (0.429, 0.903)$

plot2a.pdf

Example 1 (continued)

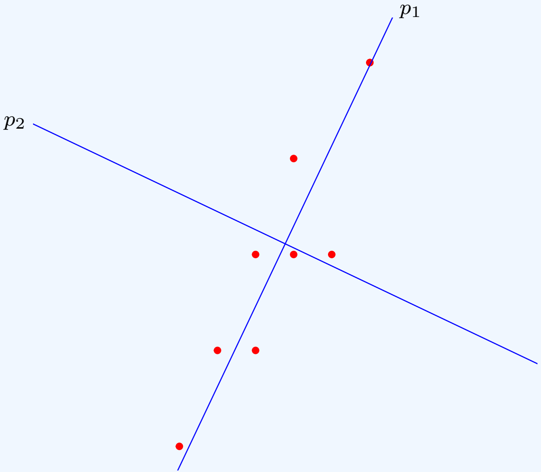


$\mathbf{v}_1 = (0.429, 0.903)$

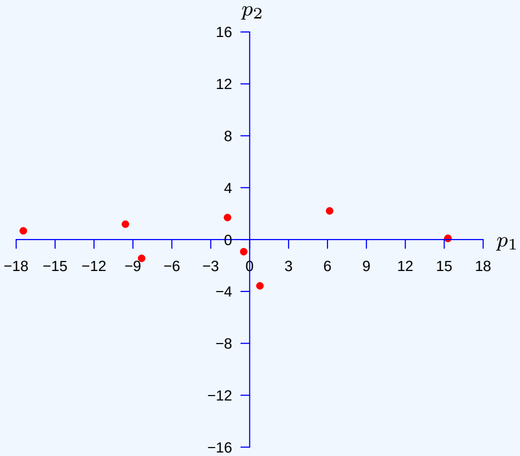
$\mathbf{v}_2 = (-0.903, 0.429)$

plot2.pdf

Example 1 (continued)



Example 1 (continued)



Principal components

Example 1 (continued)

The two principal components are

$$\hat{\lambda}_{i1} = 0.429\tilde{x}_{i1} + 0.903\tilde{x}_{i2}$$
$$\hat{\lambda}_{i2} = -0.903\tilde{x}_{i1} + 0.429\tilde{x}_{i2}$$

	i	$\tilde{x}_{i1}$	$\tilde{x}_{i2}$	$\hat{\lambda}_{i1}$	$\hat{\lambda}_{i2}$
	1	−2.27	−8.14	−8.33	−1.45
	2	−2.27	−0.81	−1.71	1.70
	3	−8.09	−15.47	−17.45	0.67
	4	−5.18	−8.14	−9.58	1.19
case	5	0.65	−0.81	−0.46	−0.93
	6	0.65	6.52	6.16	2.21
	7	6.48	13.85	15.28	0.09
	8	3.56	−0.81	0.79	−3.57
	9	6.48	13.85	15.28	0.09

Eigen-decomposition

It follows that the sample covariance matrix equals

$$\mathbf{S} = \tilde{\mathbf{X}}^T\tilde{\mathbf{X}}/N = \left(\mathbf{U}\mathbf{D}\mathbf{V}^T\right)^T\mathbf{U}\mathbf{D}\mathbf{V}^T/N = \mathbf{V}\mathbf{D}^2\mathbf{V}^T/N = \mathbf{V}\boldsymbol{\Delta}\mathbf{V}^T$$

where

- the columns of $\mathbf{V} = [\,\mathbf{v}_1 \ \ldots \ \mathbf{v}_p\,]$ are now called the eigenvectors of covariance matrix $\mathbf{S}$
- $\boldsymbol{\Delta} = \mathbf{D}^2/N$ is a $p \times p$ diagonal matrix with diagonal elements

  $$\delta_1 = d_1^2/N \ \geq \ \delta_2 = d_2^2/N \ \geq \ \ldots \ \geq \ \delta_p = d_p^2/N \ \geq \ 0$$

  known as the eigenvalues of covariance matrix $\mathbf{S}$ (the variances of the principal components)

Eigen-decomposition

Example 1 (continued)

$$\mathbf{S} = \frac{1}{9}\begin{bmatrix} -2.27 & -8.14 \\ -2.27 & -0.81 \\ -8.09 & -15.47 \\ -5.18 & -8.14 \\ 0.65 & -0.81 \\ 0.65 & 6.52 \\ 6.48 & 13.85 \\ 3.56 & -0.81 \\ 6.48 & 13.85 \end{bmatrix}^T \begin{bmatrix} -2.27 & -8.14 \\ -2.27 & -0.81 \\ -8.09 & -15.47 \\ -5.18 & -8.14 \\ 0.65 & -0.81 \\ 0.65 & 6.52 \\ 6.48 & 13.85 \\ 3.56 & -0.81 \\ 6.48 & 13.85 \end{bmatrix} = \begin{bmatrix} 22.22 & 40.87 \\ 40.87 & 88.89 \end{bmatrix}$$

$$\mathbf{S} = \begin{bmatrix} 22.22 & 40.87 \\ 40.87 & 88.89 \end{bmatrix} = \begin{bmatrix} 0.43 & -0.90 \\ 0.90 & 0.43 \end{bmatrix} \begin{bmatrix} 108.30 & 0.00 \\ 0.00 & 2.81 \end{bmatrix} \begin{bmatrix} 0.43 & 0.90 \\ -0.90 & 0.43 \end{bmatrix}$$

Total variance explained

Can most of the total variance be explained by a smaller than p number of principal components?

Total variance

$$\sum_{j=1}^{p} s_j^2 = \text{tr}(\mathbf{S}) = \text{tr}(\mathbf{V}\mathbf{\Delta}\mathbf{V}^T) = \text{tr}(\mathbf{\Delta}\mathbf{V}^T\mathbf{V}) = \text{tr}(\mathbf{\Delta}) = \sum_{j=1}^{p} \delta_j$$

The percentage of total variance explained by the jth principal component is

$$\{\delta_j/\text{tr}(\mathbf{\Delta})\} \times 100\%$$

The cumulative percentage of total variance explained by the first q principal components is

$$\{(\delta_1 + \ldots + \delta_q)/\text{tr}(\mathbf{\Delta})\} \times 100\%$$

Total variance explained

Example 1 (continued)

	i	$\tilde{x}_{i1}$	$\tilde{x}_{i2}$	$\hat{\lambda}_{i1}$	$\hat{\lambda}_{i2}$
	1	-2.27	-8.14	-8.33	-1.45
	2	-2.27	-0.81	-1.71	1.70
	3	-8.09	-15.47	-17.45	0.67
	4	-5.18	-8.14	-9.58	1.19
case	5	0.65	-0.81	-0.46	-0.93
	6	0.65	6.52	6.16	2.21
	7	6.48	13.85	15.28	0.09
	8	3.56	-0.81	0.79	-3.57
	9	6.48	13.85	15.28	0.09

Eigenvalues $\delta_1 = 108.30$ and $\delta_2 = 2.81$

Total variance explained

The number of principal components to be extracted is equal to the number of principal components with a cumulative percentage of total variance explained at least as high as a prespecified percentage

Example 1 (continued)

Suppose it is desired to explain at least 80% of the total variance

The percentage of total variance explained by the first principal component is

$$\frac{108.30}{108.30 + 2.81} \times 100\% \approx 97\%$$

According to this criterion, one principal component should be extracted

Standardization

Let $S = \text{diag}\{s_1, s_2, \ldots, s_p\}$

The inverse of S is $S^{-1} = \text{diag}\left\{\frac{1}{s_1}, \frac{1}{s_2}, \ldots, \frac{1}{s_p}\right\}$ because $SS^{-1} = \mathbf{I}$

The standardized data matrix is

$$\mathbf{Z} = \tilde{\mathbf{X}}S^{-1}$$

The covariance matrix of the standardized features is the correlation matrix

$$\mathbf{R} = \mathbf{Z}^T\mathbf{Z}/N = (\tilde{\mathbf{X}}S^{-1})^T\tilde{\mathbf{X}}S^{-1}/N = S^{-1}(\tilde{\mathbf{X}}^T\tilde{\mathbf{X}}/N)S^{-1} = S^{-1}\mathbf{S}S^{-1}$$

Standardization

Example 1 (continued)

The standardized data matrix

$$\mathbf{Z} = \begin{bmatrix} -2.27 & -8.14 \\ -2.27 & -0.81 \\ -8.09 & -15.47 \\ -5.18 & -8.14 \\ 0.65 & -0.81 \\ 0.65 & 6.52 \\ 6.48 & 13.85 \\ 3.56 & -0.81 \\ 6.48 & 13.85 \end{bmatrix} \begin{bmatrix} 4.71 & 0.00 \\ 0.00 & 9.43 \end{bmatrix}^{-1} = \begin{bmatrix} -0.48 & -0.86 \\ -0.48 & -0.09 \\ -1.72 & -1.64 \\ -1.10 & -0.86 \\ 0.14 & -0.09 \\ 0.14 & 0.69 \\ 1.37 & 1.47 \\ 0.76 & -0.09 \\ 1.37 & 1.47 \end{bmatrix}$$

The correlation matrix

$$\mathbf{R} = \mathbf{Z}^T\mathbf{Z}/9 = \begin{bmatrix} 1.00 & 0.92 \\ 0.92 & 1.00 \end{bmatrix}$$

Singular value decomposition of $\mathbf{Z}$

Example 1 (continued)

$$\mathbf{Z} = \begin{bmatrix} -0.48 & -0.86 \\ -0.48 & -0.09 \\ -1.72 & -1.64 \\ -1.10 & -0.86 \\ 0.14 & -0.09 \\ 0.14 & 0.69 \\ 1.37 & 1.47 \\ 0.76 & -0.09 \\ 1.37 & 1.47 \end{bmatrix} = \begin{bmatrix} -0.23 & 0.32 \\ -0.10 & -0.33 \\ -0.57 & -0.06 \\ -0.33 & -0.20 \\ 0.01 & 0.19 \\ 0.14 & -0.46 \\ 0.48 & -0.08 \\ 0.11 & 0.70 \\ 0.48 & -0.08 \end{bmatrix} \begin{bmatrix} 4.16 & 0.00 \\ 0.00 & 0.85 \end{bmatrix} \begin{bmatrix} 0.71 & 0.71 \\ 0.71 & -0.71 \end{bmatrix}$$

Singular value decomposition of $\mathbf{Z}$

Example 1 (continued)

Principal component scores

$$\tilde{\mathbf{\Lambda}} = \begin{bmatrix} -0.48 & -0.86 \\ -0.48 & -0.09 \\ -1.72 & -1.64 \\ -1.10 & -0.86 \\ 0.14 & -0.09 \\ 0.14 & 0.69 \\ 1.37 & 1.47 \\ 0.76 & -0.09 \\ 1.37 & 1.47 \end{bmatrix} \begin{bmatrix} 0.71 & 0.71 \\ 0.71 & -0.71 \end{bmatrix} = \begin{bmatrix} -0.23 & 0.32 \\ -0.10 & -0.33 \\ -0.57 & -0.06 \\ -0.33 & -0.20 \\ 0.01 & 0.19 \\ 0.14 & -0.46 \\ 0.48 & -0.08 \\ 0.11 & 0.70 \\ 0.48 & -0.08 \end{bmatrix} \begin{bmatrix} 4.16 & 0.00 \\ 0.00 & 0.85 \end{bmatrix} = \begin{bmatrix} -0.95 & 0.27 \\ -0.40 & -0.28 \\ -2.37 & -0.05 \\ -1.39 & -0.17 \\ 0.04 & 0.16 \\ 0.59 & -0.39 \\ 2.01 & -0.07 \\ 0.47 & 0.60 \\ 2.01 & -0.07 \end{bmatrix}$$

Eigen-decomposition of $\mathbf{R}$

Example 1 (continued)

$$\mathbf{R} = \begin{bmatrix} 1.00 & 0.92 \\ 0.92 & 1.00 \end{bmatrix} = \begin{bmatrix} 0.71 & 0.71 \\ 0.71 & -0.71 \end{bmatrix} \begin{bmatrix} 1.92 & 0.00 \\ 0.00 & 0.08 \end{bmatrix} \begin{bmatrix} 0.71 & 0.71 \\ 0.71 & -0.71 \end{bmatrix}$$

Total variance: $\text{tr}(\mathbf{R}) = p$

The percentage of total variance explained by the first principal component is

$$\frac{1.92}{1.92 + 0.08} \times 100\% \approx 96\%$$

Scree test

Example 2

6 standardized features and $n = 1000$

The first three are measurements of spacial ability
The last three are measurements of verbal ability

Correlation matrix

$$\begin{bmatrix} 1.00 & & & & & \\ 0.75 & 1.00 & & & & \\ 0.81 & 0.78 & 1.00 & & & \\ 0.18 & 0.25 & 0.25 & 1.00 & & \\ 0.08 & 0.15 & 0.15 & 0.90 & 1.00 & \\ 0.14 & 0.21 & 0.20 & 0.87 & 0.84 & 1.00 \end{bmatrix}$$

Scree test

Example 2 (continued)

Component	Eigenvalue	PVE	CPVE
1	3.195	53.256	53.256
2	2.118	35.296	88.552
3	.248	4.130	92.682
4	.186	3.107	95.789
5	.163	2.715	98.504
6	.090	1.496	100.000

In a so-called scree plot, the eigenvalues of the principal components are plotted against the rank numbers of the principal components

Scree test

Example 2 (continued)

The number of principal components to be extracted is equal to the number of eigenvalues greater than the elbow in the scree plot

Interpretation

The component matrix might help in interpreting the extracted principal components → which features play a role?

The elements of the component matrix are

- the correlations between the standardized features and the extracted principal components
- the standardized regression coefficients from the regression of the standardized features on the extracted principal components

		Component		
		1	$\dots$	q
Standardized feature	1	r_{11}	$\dots$	r_{1q}
	2	r_{21}	$\dots$	r_{2q}
	$\vdots$	$\vdots$		$\vdots$
	p	r_{p1}	$\dots$	r_{pq}

Interpretation

Example 2 (continued)

	Component	
	1	2
Feature 1	.630	.678
Feature 2	.682	.609
Feature 3	.688	.633
Feature 4	.825	-.504
Feature 5	.755	-.593
Feature 6	.781	-.531

Principal component regression

Prediction of y from the first $m < p$ principal components of $\tilde{x}_1, \ldots, \tilde{x}_p$

Multiple regression (interval response): $y = g(\hat{\lambda}_1, \ldots, \hat{\lambda}_m) + \varepsilon$

Binary logistic regression: $\pi = \dfrac{\exp\{g(\hat{\lambda}_1, \ldots, \hat{\lambda}_m)\}}{1 + \exp\{g(\hat{\lambda}_1, \ldots, \hat{\lambda}_m)\}}$

By estimating only $m + 1$ coefficients, overfitting can be mitigated

Assumption: $\hat{\lambda}_1, \ldots, \hat{\lambda}_m$ are sufficient to predict y

The number of principal components m can be determined by cross-validation

Principal component regression

Linear prediction of y from the first $m < p$ principal components of $\tilde{x}_1, \ldots, \tilde{x}_p$

$$
\begin{aligned}
g(\hat{\lambda}_1, \ldots, \hat{\lambda}_m) &= \alpha_0 + \alpha_1 \hat{\lambda}_1 + \ldots + \alpha_m \hat{\lambda}_m = \alpha_0 + \sum_{j=1}^{m} \alpha_j \hat{\lambda}_j = \alpha_0 + \sum_{j=1}^{m} \alpha_j (v_{1j}\tilde{x}_1 + \ldots + v_{kj}\tilde{x}_p) \\
&= \alpha_0 + \left(\sum_{j=1}^{m} \alpha_j v_{1j} \right) \tilde{x}_1 + \ldots + \left(\sum_{j=1}^{m} \alpha_j v_{pj} \right) \tilde{x}_p = f(\tilde{x}_1, \ldots, \tilde{x}_p)
\end{aligned}
$$

So

$$
f(\tilde{x}_1, \ldots, \tilde{x}_p) = \beta_0 + \beta_1 \tilde{x}_1 + \ldots + \beta_p \tilde{x}_p, \text{ where } \beta_0 = \alpha_0, \beta_1 = \sum_{j=1}^{m} \alpha_j v_{1j}, \ \ldots, \ \beta_p = \sum_{j=1}^{m} \alpha_j v_{pj}
$$