

Principle Components Analysis

Inner Products

Row vector $\mathbf{a} = (a_1, a_2, \dots, a_n)$

Column vector $\mathbf{b}^T = \begin{pmatrix} b_1 \\ b_2 \\ \cdot \\ \cdot \\ \cdot \\ b_n \end{pmatrix}$

$$\mathbf{a} \cdot \mathbf{b} = \sum_{i=1}^n a_i b_i = \mathbf{a} \mathbf{b}^T = (a_1, a_2, \dots, a_n) \begin{pmatrix} b_1 \\ b_2 \\ \cdot \\ \cdot \\ \cdot \\ b_n \end{pmatrix}$$

Orthogonality and norm

$\mathbf{a} \cdot \mathbf{b} = 0$ $\mathbf{a}$ and $\mathbf{b}$ are **orthogonal** vectors

Norm $\|\mathbf{a}\|_2^2 \doteq \mathbf{a} \cdot \mathbf{a} = \sum_{i=1} a_i^2$

Unit vector $\|\mathbf{a}\|_2 = 1$

matrix-vector product

$$A = \begin{pmatrix} a_{1,1}, a_{1,2}, \dots, a_{1,m} \\ a_{2,1}, a_{2,2}, \dots, a_{2,m} \\ \dots \\ \dots \\ a_{n,1}, a_{n,2}, \dots, a_{n,m} \end{pmatrix} = \begin{pmatrix} \mathbf{a}_1 \\ \mathbf{a}_2 \\ \cdot \\ \cdot \\ \cdot \\ \mathbf{a}_n \end{pmatrix}$$

$$A\mathbf{b}^T = \begin{pmatrix} \mathbf{a}_1\mathbf{b}^T \\ \mathbf{a}_2\mathbf{b}^T \\ \dots \\ \dots \\ \mathbf{a}_n\mathbf{b}^T \end{pmatrix} = \begin{pmatrix} \sum_{i=1}^m a_{1,i}b_i \\ \sum_{i=1}^m a_{2,i}b_i \\ \dots \\ \dots \\ \sum_{i=1}^m a_{n,i}b_i \end{pmatrix}$$

matrix-matrix product

$$A = \begin{pmatrix} a_{1,1}, a_{1,2}, \dots, a_{1,m} \\ a_{2,1}, a_{2,2}, \dots, a_{2,m} \\ \dots \\ \dots \\ a_{n,1}, a_{n,2}, \dots, a_{n,m} \end{pmatrix} = \begin{pmatrix} \mathbf{a}_1 \\ \mathbf{a}_2 \\ \cdot \\ \cdot \\ \cdot \\ \mathbf{a}_n \end{pmatrix}$$

$$B = \begin{pmatrix} b_{1,1}, b_{1,2}, \dots, b_{1,l} \\ b_{2,1}, b_{2,2}, \dots, b_{2,l} \\ \dots \\ \dots \\ b_{m,1}, b_{m,2}, \dots, b_{m,l} \end{pmatrix} = (\mathbf{b}_1^T, \mathbf{b}_2^T, \dots, \mathbf{b}_l^T)$$

$$AB = \begin{pmatrix} (\mathbf{a}_1 \cdot \mathbf{b}_1), (\mathbf{a}_1 \cdot \mathbf{b}_2), \dots, (\mathbf{a}_1 \cdot \mathbf{b}_l) \\ (\mathbf{a}_2 \cdot \mathbf{b}_1), (\mathbf{a}_2 \cdot \mathbf{b}_2), \dots, (\mathbf{a}_2 \cdot \mathbf{b}_l) \\ \dots \\ \dots \\ (\mathbf{a}_n \cdot \mathbf{b}_1), (\mathbf{a}_n \cdot \mathbf{b}_2), \dots, (\mathbf{a}_n \cdot \mathbf{b}_l) \end{pmatrix}$$

diagonal matrices

$$D\mathbf{b}^T = \begin{pmatrix} \lambda_1, 0, 0, \dots, 0 \\ 0, \lambda_2, 0, \dots, 0 \\ 0, 0, \lambda_3, \dots, 0 \\ \dots \\ \dots \\ 0, 0, 0, \dots, \lambda_n \end{pmatrix} \begin{pmatrix} b_1 \\ b_2 \\ \cdot \\ \cdot \\ \cdot \\ b_n \end{pmatrix} = \begin{pmatrix} \lambda_1 b_1 \\ \lambda_2 b_2 \\ \cdot \\ \cdot \\ \cdot \\ \lambda_n b_n \end{pmatrix}$$

$$I\mathbf{b}^T = \begin{pmatrix} 1, 0, 0, \dots, 0 \\ 0, 1, 0, \dots, 0 \\ 0, 0, 1, \dots, 0 \\ \dots \\ \dots \\ 0, 0, 0, \dots, 1 \end{pmatrix} \begin{pmatrix} b_1 \\ b_2 \\ \cdot \\ \cdot \\ \cdot \\ b_n \end{pmatrix} = \begin{pmatrix} b_1 \\ b_2 \\ \cdot \\ \cdot \\ \cdot \\ b_n \end{pmatrix}$$

Orthonormal Matrices

A is a square matrix ($n \times n$)

$$A = \begin{pmatrix} \mathbf{a}_1 \\ \mathbf{a}_2 \\ \vdots \\ \mathbf{a}_n \end{pmatrix} \quad A^T = (\mathbf{a}_1^T, \mathbf{a}_2^T, \dots, \mathbf{a}_n^T)$$

$$AA^T = I$$

The rows of **A** define an orthonormal basis

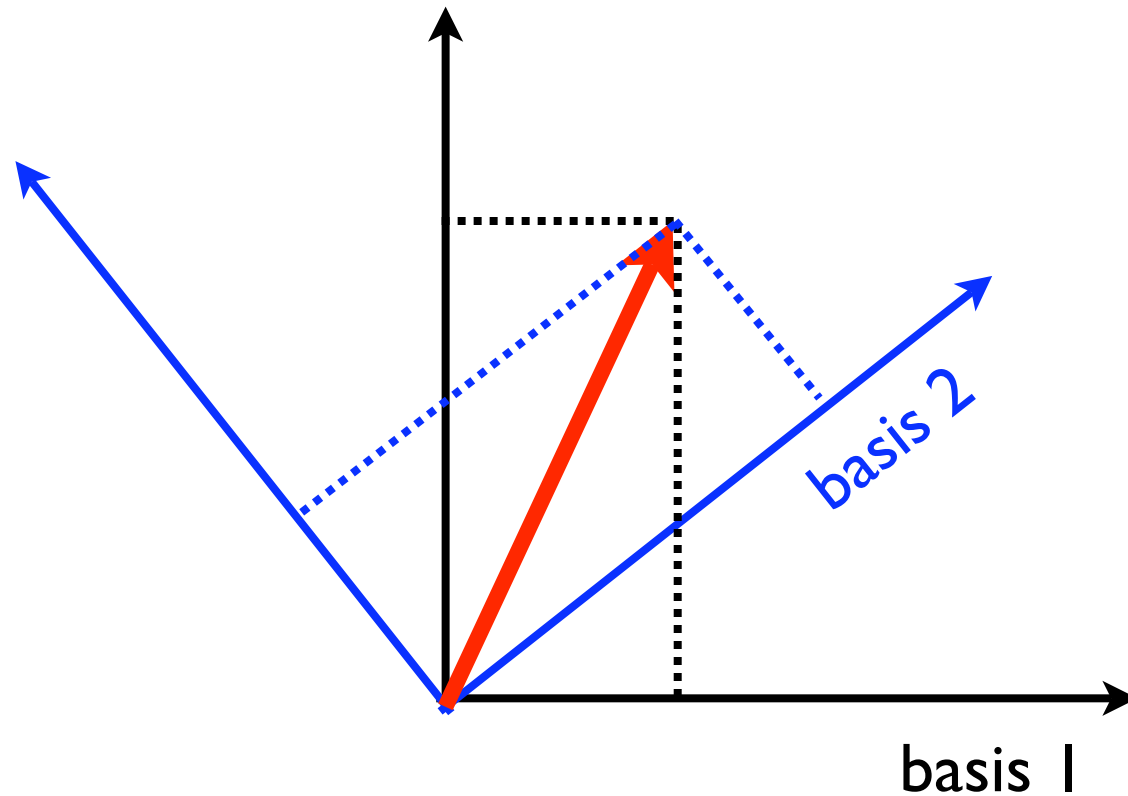
$$\forall i \neq j, \quad \mathbf{a}_i \cdot \mathbf{a}_i = \|\mathbf{a}\|_2^2 = 1, \quad \mathbf{a}_i \cdot \mathbf{a}_j = 0$$

Orthonormal matrices and vector bases

- A set of n orthogonal unit vectors in $\mathbb{R}^n$ defines an orthonormal basis.
- Multiplying a vector by an orthonormal matrix corresponds to expressing it in terms of the orthonormal basis.

Changing basis in $\mathbb{R}^2$

basis = coordinate system



Eigenvectors and Eigenvalues

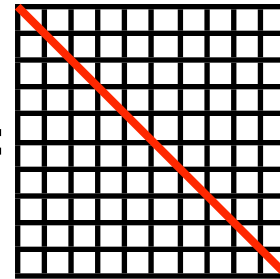
the vector **a** is an **eigenvector** of the matrix **M** with **eigenvalue** λ if

$$Ma = \lambda a$$

In words: the application of **M** to **a** amounts to changing the **length** of **a** by a factor of λ without changing **a**'s **direction**

Decomposing Symmetric Matrices

A symmetric matrix **M** =



M can be written in the form

$$M = A^T \begin{pmatrix} \lambda_1, 0, 0, \dots, 0 \\ 0, \lambda_2, 0, \dots, 0 \\ 0, 0, \lambda_3, \dots, 0 \\ \dots \\ \dots \\ 0, 0, 0, \dots, \lambda_n \end{pmatrix} A$$

A is an orthonormal matrix consisting of the eigenvectors of **M**

Interpretation of the decomposition

- the operation $A^T D A \mathbf{a}$ equals:
 1. transform $\mathbf{a}$ into basis defined by A
 2. multiply each coordinate i by λ_i
 3. transform back to original basis

Principle components of covariance matrices

$$\text{cov}(\mathbf{x}) = \begin{pmatrix} \text{var}(x_1), & \text{cov}(x_1, x_2), \dots & \text{cov}(x_1, x_n) \\ \text{cov}(x_2, x_1), & \text{var}(x_2), \dots & \text{cov}(x_2, x_n) \\ & \dots & \\ & \dots & \\ \text{cov}(x_n, x_1), & \text{cov}(x_n, x_2), \dots & \text{var}(x_n) \end{pmatrix}$$

Symmetric matrix because $\text{cov}(x_i, x_j) = \text{cov}(x_j, x_i)$

Can be expressed as $\text{cov}(\mathbf{x}) = \mathbf{A}^T \mathbf{D} \mathbf{A}$

Interpretation of principle components

- distribution of random vector $\mathbf{x}$ defines covariance matrix $\text{cov}(\mathbf{x})$
- decomposition $\text{cov}(\mathbf{x}) = \mathbf{A}^T \mathbf{D} \mathbf{A}$ changes the coordinate system of $\mathbf{x}$
- defines a new random vector $\mathbf{y} = \mathbf{A} \mathbf{x}$
- $\text{cov}(\mathbf{y}) = \mathbf{D}$
- $\text{var}(y_i) = \lambda_i$, $\forall i \neq j: \text{cov}(y_i, y_j) = 0$

The observations matrix

$$\begin{array}{c} \text{n observations} \end{array} \begin{pmatrix} \text{p variables} \\ x_{1,1}, x_{1,2}, \dots, x_{1,p} \\ x_{2,1}, x_{2,2}, \dots, x_{2,p} \\ \dots \\ \dots \\ x_{n,1}, x_{n,2}, \dots, x_{n,p} \end{pmatrix} = \begin{pmatrix} \mathbf{x}_1 \\ \mathbf{x}_2 \\ \cdot \\ \cdot \\ \cdot \\ \mathbf{x}_n \end{pmatrix}$$

Calculating the cov matrix

$$\bar{\mathbf{x}} = \frac{1}{n} \sum_{i=1}^n \mathbf{x}_i$$

Outer product

$$\frac{1}{n} \sum_{i=1}^n \mathbf{x}_i^T \mathbf{x}_i$$

$$\text{Cov}(x, y) = E(xy) - E(x)E(y)$$

$$\text{COV} = \frac{1}{n} \sum_{i=1}^n \mathbf{x}_i^T \mathbf{x}_i - \bar{\mathbf{x}}^T \bar{\mathbf{x}}$$

Calculating PCA

- Find all eigenvectors and eigenvalues of COV
- Sort by order of decreasing eigenvalue.

matlab: `princomp`

- `[COEFF, SCORE, latent, tsquare] = princomp(X)`
- `COEFF` = eigen vectors (orthonormal matrix)
- `latent` = eigen values
- `SCORE` = samples in `X` represented in `COEFF` basis
- `tsquare` - t-square test for outliers