Lecture 13: Principal components analysis (PCA)

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High-Dimensional Data

- High-Dimensions = Lot of Features

Surveys Netflix

	movie 1	movie 2	movie 3	movie 4	movie 5	movie 6
Tom	5	?	?	1	3	?
George	?	?	3	1	2	5
Susan	4	3	1	?	5	1
Beth	4	3	?	2	4	2

Food preference

	kale	taco bell	sashimi	pop tarts
Alice	10	1	2	7
Bob	7	2	1	10
Carolyn	2	9	7	3
Dave	3	6	10	2

- PCA: Unsupervised learning techniques to extract hidden dimensional structure from high dimensional dataset
  - Visualization
  - Efficient use of resources.
  - Statistical: lower dimension --> better generalization.
  - Further processing for other machine learning algorithm.

Motivating problem

- Friends’ preferences of four different food choice.
- Dimension of data points: 4
- Number of data points: 4

Can we visualize the data in less than 4 dimension?

	kale	taco bell	sashimi	pop tarts
Alice	10	1	2	7
Bob	7	2	1	10
Carolyn	2	9	7	3
Dave	3	6	10	2

Table 1: Your friends’ ratings of four different foods.

Motivating problem

- Each row of the data can be expressed approximately:

	kale	taco bell	sashimi	pop tarts
Alice	10	1	2	7
Bob	7	2	1	10
Carolyn	2	9	7	3
Dave	3	6	10	2

Table 1: Your friends' ratings of four different foods.

Name	(a_1, a_2)
Alice	$(1,\ 1)$
Bob	$(1,\ -1)$
Carolyn	$(-1,\ -1)$
Dave	$(-1,\ 1)$

Table 1: Values of (a_1, a_2) for each person

$$\bar{\mathbf{x}} + a_1\mathbf{v}_1 + a_2\mathbf{v}_2,$$

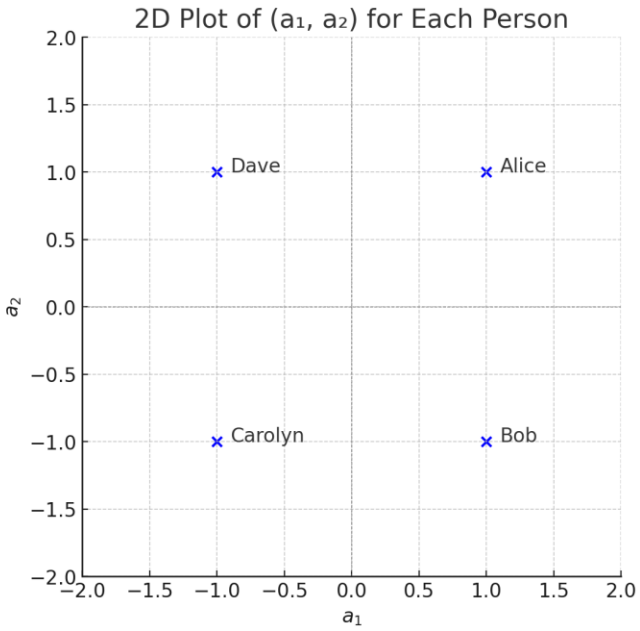
where

$$\bar{\mathbf{x}} = (5.5, 4.5, 5, 5.5)$$

is the average of the data points,

$$\mathbf{v}_1 = (3, -3, -3, 3),$$

$$\mathbf{v}_2 = (1, -1, 1, -1),$$



The role of PCA

- Reduce the dimensionality of data points (eg. 4 to 2):
- Given a list of m n-dimensional vectors (data points),

$$x_1, x_2, \ldots, x_m \in R^n$$

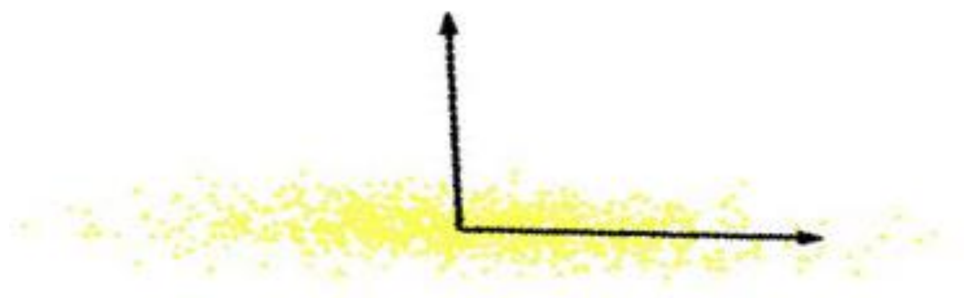
For each vector x_i, express it as linear combinations of k n-dimensional vectors $v_1, \ldots, v_n \in R^n$ such that

$$x_i \approx \sum_{j \in 1}^{k} a_{ij} v_j$$

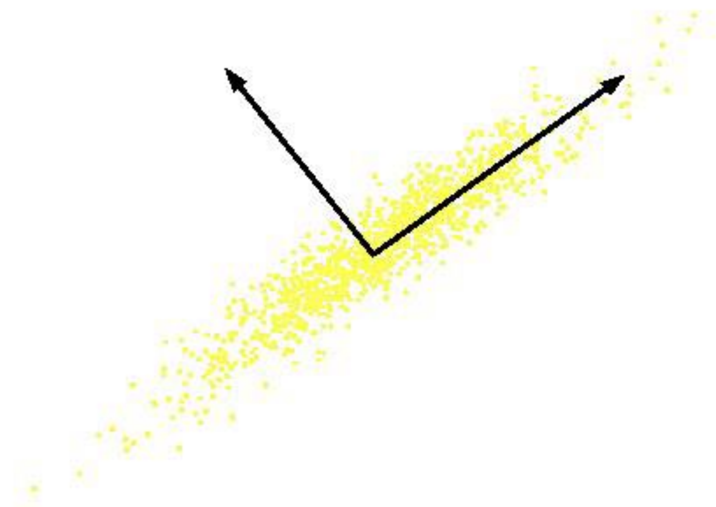
Dimension reduction: n → k, which is smaller than n.

PCA

- PCA is an orthogonal projection or transformation of the data into a possible lower dimensional subspace so that **the variance of the projected data is maximized.**



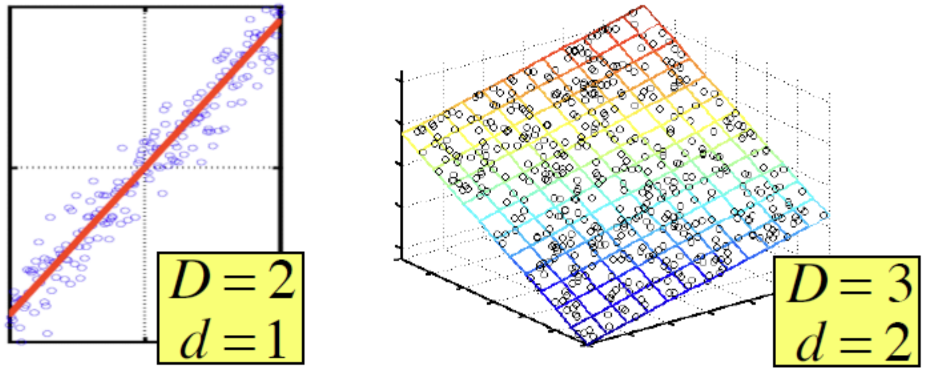
Only one relevant feature



Both features are relevant, but

PCA

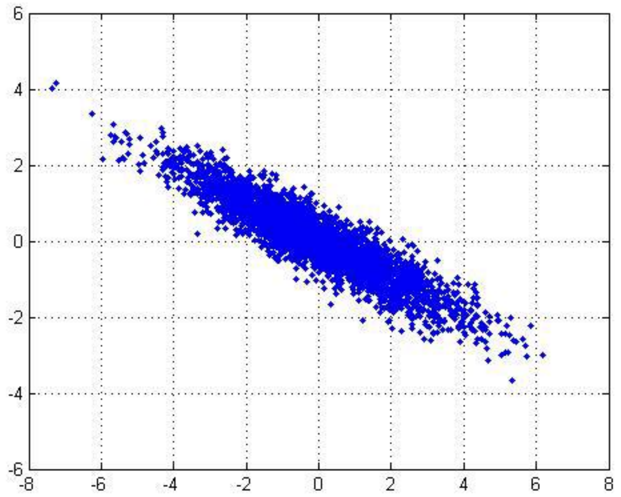
- The goal is to identify the axes or subspace the high-dimensional data should be projected into.



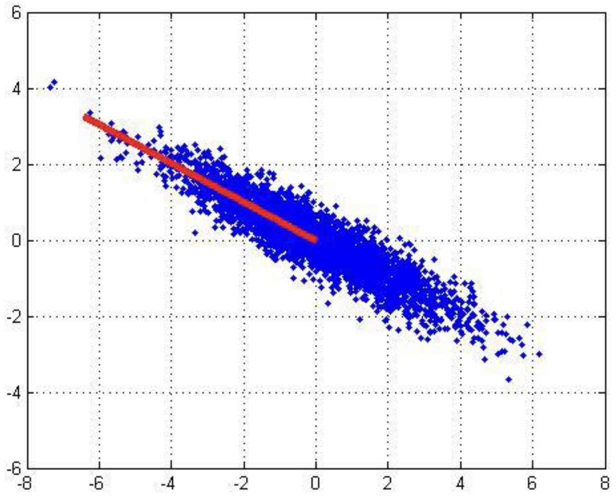
Does the data mostly lie in a subspace?
If so, what is its dimensionality?

Maximize the variance

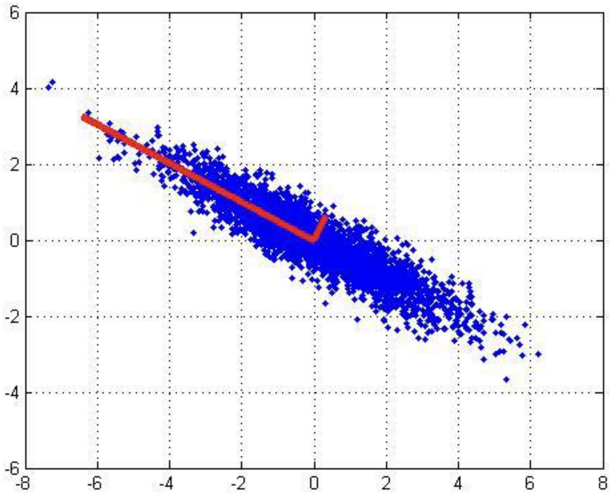
- Why maximize the variance of the projected data?



2D Gaussian dataset



1st principle component



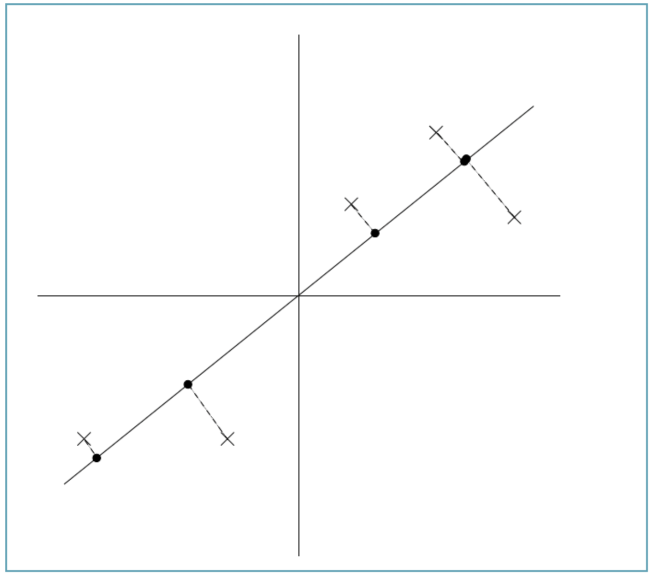
2nd principle component

Variance tells us how much information or “spread” a dataset has. In PCA, we assume directions with higher variance are more informative.

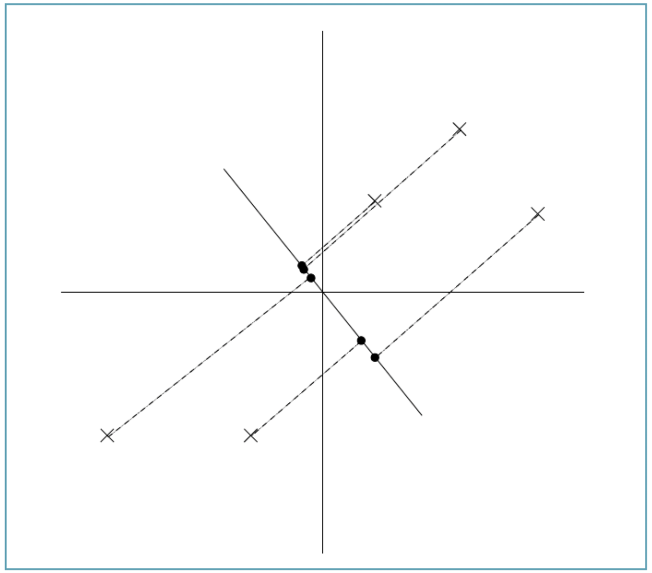
Maximize the variance

- Which of the two projections maximize the variance?

Option A



Option B



Figures from Andrew Ng
(CS229 Lecture Notes)

Maximize the variance

We want to find new axes (directions) to project our data such that:

- The projected data has **maximum variance**.
- The new features (called principal components) are **uncorrelated**.

	kale	taco bell	sashimi	pop tarts
Alice	10	1	2	7
Bob	7	2	1	10
Carolyn	2	9	7	3
Dave	3	6	10	2

Table 1: Your friends' ratings of four different foods.

Step 1: center the data matrix
Step 2: compute the covariance matrix of the centered data
Step 3: select top k principal components/features

Step 1 and step 2

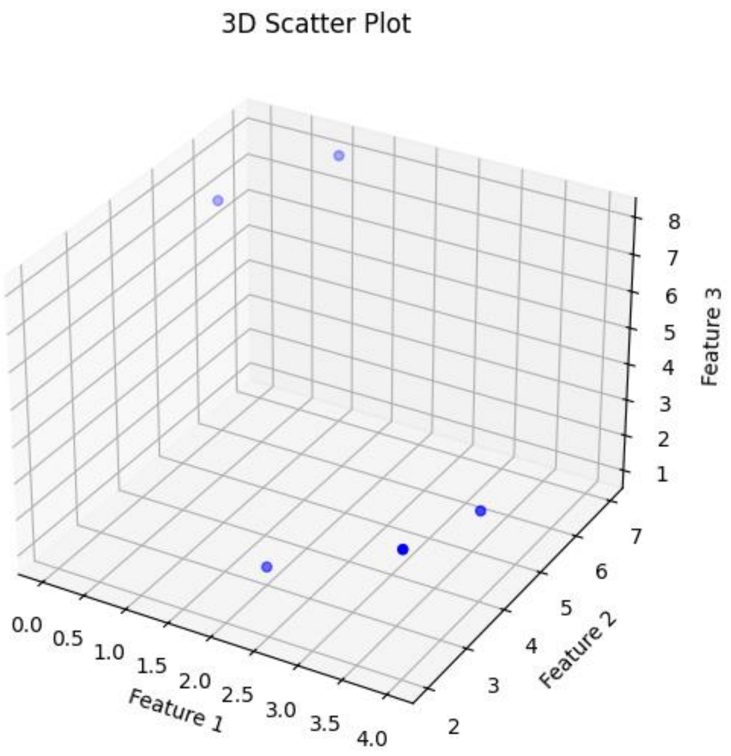
- Center the data

$$X_c = X - \bar{X}$$

- Example:

Consider the following dataset with 5 samples and 3 features:

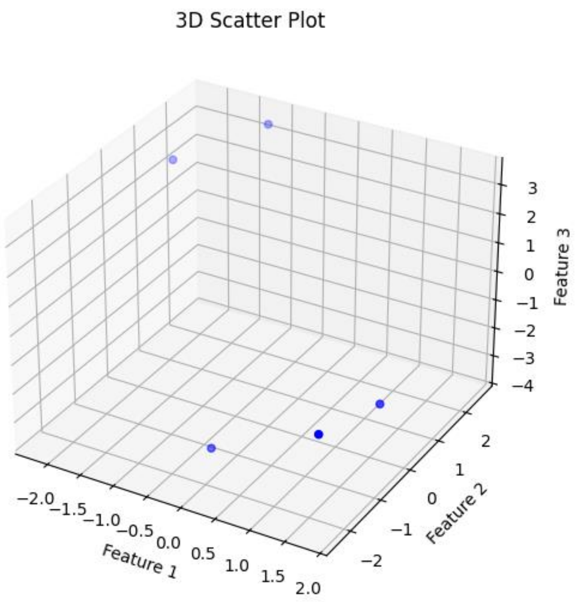
$$X = \begin{bmatrix} 2 & 3 & 1 \\ 4 & 2 & 4 \\ 4 & 4 & 3 \\ 0 & 6 & 7 \\ 1 & 7 & 8 \end{bmatrix}$$



Mean of each feature

- Centered data matrix

$$X_c = \begin{bmatrix} -0.2 & -1.4 & -3.6 \\ 1.8 & -2.4 & -0.6 \\ 1.8 & -0.4 & -1.6 \\ -2.2 & 1.6 & 2.4 \\ -1.2 & 2.6 & 3.4 \end{bmatrix}$$



Step 2: compute the covariance matrix of the centered data (use the transposed.)

np.cov(M_c.T)

The covariance matrix K is given by:

$$K = \frac{1}{n-1} X_c^\top X_c$$

$$\begin{bmatrix} 3.2 & -2.85 & -3.15 \\ -2.85 & 4.3 & 4.95 \\ -3.15 & 4.95 & 8.3 \end{bmatrix}$$

Eigenvalue and eigenvectors of a matrix

Let A be a $n \times n$ matrix.

- $\vec{x} \neq 0$ is an *eigenvector* of A if there is a scalar λ such that

$$A\vec{x} = \lambda\vec{x}$$

- the corresponding λ is called the *eigenvalue*.

- Example: find the eigenvalue and eigenvector of A.

$$A = \begin{bmatrix} 4 & 2 \\ 1 & 3 \end{bmatrix}$$

Eigenvalue and eigenvectors of a matrix

Eigenvalue and eigenvectors of a matrix

Diagonalizable Matrices

A $n \times n$ matrix with n linearly independent eigenvectors is said to be **diagonalizable.**

$$\boldsymbol{A}\,\boldsymbol{u_1} = \lambda_1\,\boldsymbol{u_1},$$
$$\boldsymbol{A}\,\boldsymbol{u_2} = \lambda_2\,\boldsymbol{u_2},$$
$$\ldots$$
$$\boldsymbol{A}\,\boldsymbol{u_n} = \lambda_n\,\boldsymbol{u_n},$$

In matrix form:

$$\boldsymbol{A}\,(\boldsymbol{u_1} \quad \cdots \quad \boldsymbol{u_n}) = (\lambda_1\boldsymbol{u_1} \quad \cdots \quad \lambda_n\boldsymbol{u_n}) = (\boldsymbol{u_1} \quad \cdots \quad \boldsymbol{u_n})\begin{pmatrix} \lambda_1 & 0 & 0 \\ 0 & \ddots & 0 \\ 0 & 0 & \lambda_n \end{pmatrix}$$

This corresponds to a similarity transformation

$$\boldsymbol{AU} = \boldsymbol{UD} \iff \boldsymbol{A} = \boldsymbol{UDU^{-1}}$$

PCA and eigen-decomposition of covariance matrix.

- Covariance matrix:

Property of covariance matrix:

1. It is symmetric → for symmetric matrix, eigenvectors for distinct eigenvalues are orthogonal.

2. It is real: -> All eigenvalues of a real symmetric matrix are real.

PCA and eigen-decomposition of covariance matrix.

- Eigen-decomposition of covariance matrix

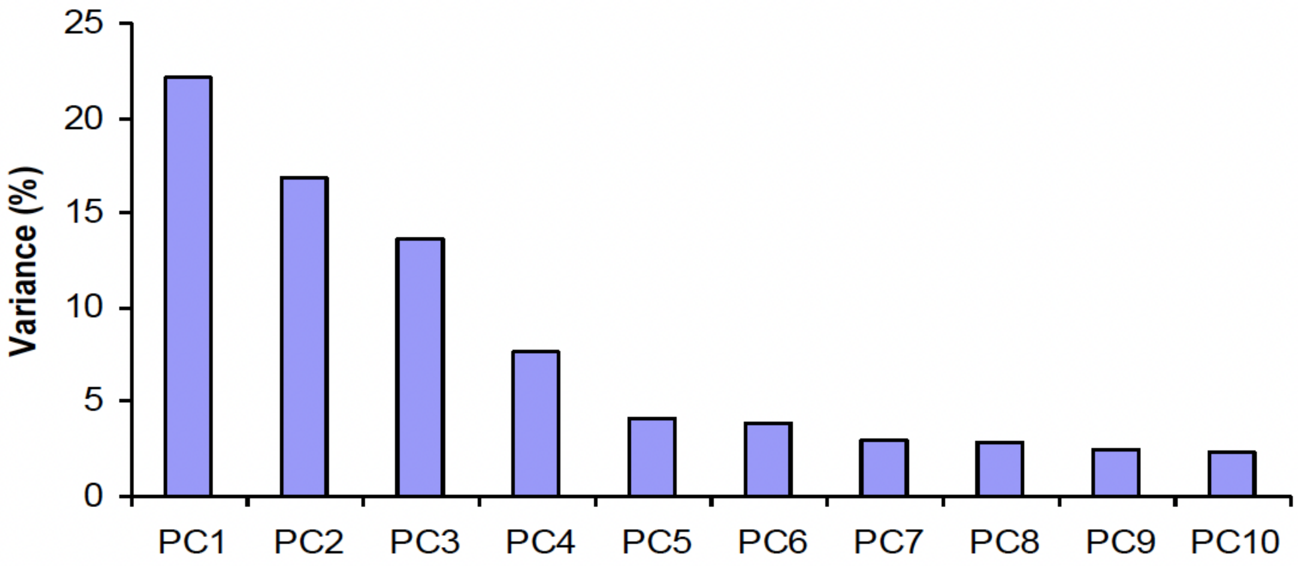
$$K = U \Lambda U^{-1}$$

$K = U \Lambda U^{-1}$

- Columns of U are *eigenvectors* of K.
- Diagonal matrix Λ are eigenvalues of K, ordered in the order of eigenvectors.

$$\Lambda = diag(\lambda_1, \lambda_2, \dots, \lambda_n)$$

- We order these eigenvectors in an order of the values of eigenvalues and called these: 1st principal component, 2nd principal component, etc.
- Where does dimensionality reduction come from?
  - Can ignore the components of lesser significance.



Example

The covariance matrix K is given by:

$$K = \frac{1}{n-1} X_c^\top X_c$$

$$\begin{bmatrix} 3.2 & -2.85 & -3.15 \\ -2.85 & 4.3 & 4.95 \\ -3.15 & 4.95 & 8.3 \end{bmatrix}$$

eigenvalues, eigenvectors = LA.eig(K)

$$\begin{bmatrix} 13.38070762 & 1.82004592 & 0.59924646 \end{bmatrix}$$

$$\begin{bmatrix} -0.38263617 & 0.77297413 & -0.50606379 \\ 0.53188845 & -0.26357343 & -0.80475072 \\ 0.75543646 & 0.57709622 & 0.31028329 \end{bmatrix}$$

PC

- Project the Data onto the Principal Components:

- If we want 2D dimension, project each centered data point into the first two pc:

$$X_c = \begin{bmatrix} -0.2 & -1.4 & -3.6 \\ 1.8 & -2.4 & -0.6 \\ 1.8 & -0.4 & -1.6 \\ -2.2 & 1.6 & 2.4 \\ -1.2 & 2.6 & 3.4 \end{bmatrix}$$

$$\begin{bmatrix} -0.38263617 & 0.77297413 & -0.50606379 \\ 0.53188845 & -0.26357343 & -0.80475072 \\ 0.75543646 & 0.57709622 & 0.31028329 \end{bmatrix}$$

Determinant of a matrix

$$\det(\mathbf{A}) = \det \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nn} \end{bmatrix}$$

$$A = \begin{bmatrix} a & b \\ c & d \end{bmatrix}$$

- Laplace expansion of the first row

$$A = \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix}$$

$$\det(A) = a_{11}(a_{22}a_{33} - a_{23}a_{32}) - a_{12}(a_{21}a_{33} - a_{23}a_{31}) + a_{13}(a_{21}a_{32} - a_{22}a_{31})$$