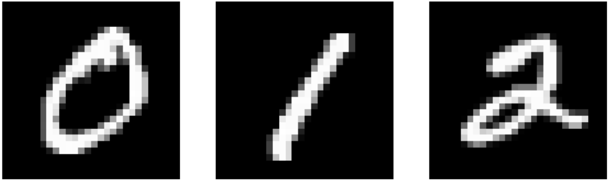
Principal component analysis

229351

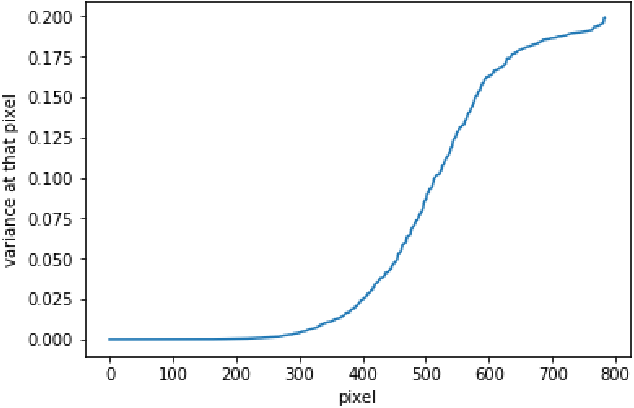
Dimensionality reduction

Why remove some of the features?

- Save storage and computation time.
- Reduce some redundancy in the data.
- Remove noises in the data.



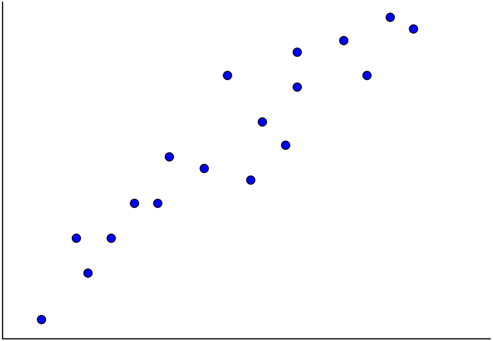
MNIST example



First 300 pixels with the lowest variance are undesirable features.

A simple case

Suppose we want to reduce from 2D data to 1D.



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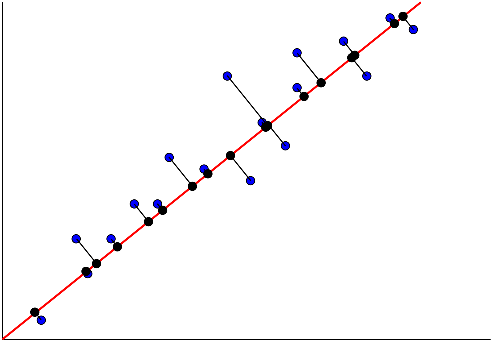
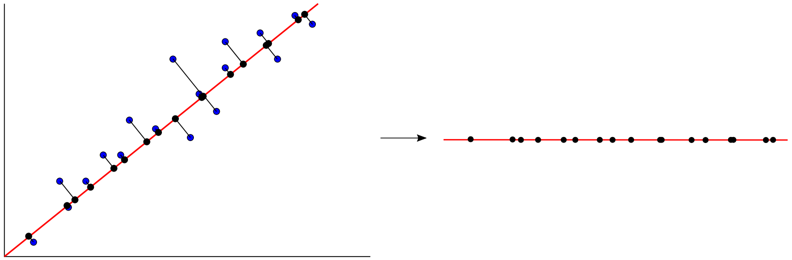


Make projections on this line.

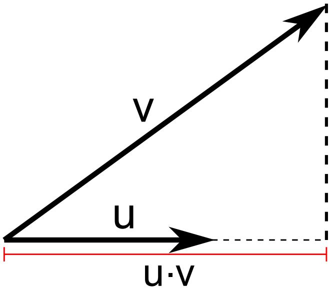
From 2D to 1D



The red line becomes the 1D axis.

Vector Projection

If we want to project a vector v in a direction of a **unit vector** u,



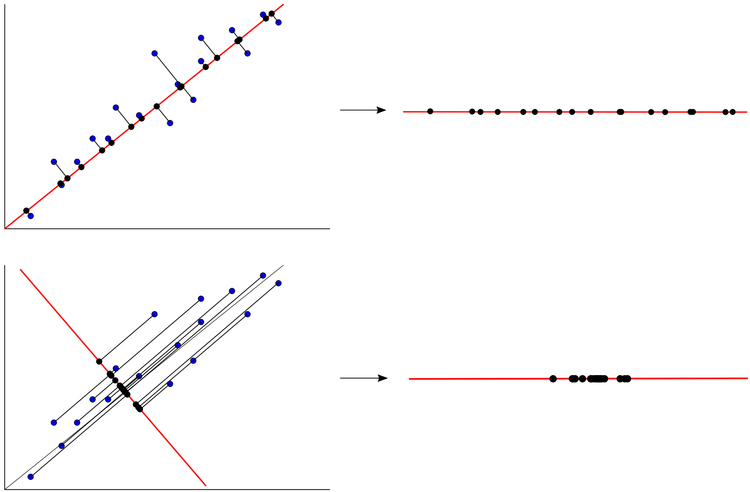
then the length of projection is $u \cdot v$.

Examples

What is the projection of $v = \begin{pmatrix} 1 \\ 2 \end{pmatrix}$ in the following directions?

- The x axis.
- The direction of $u = \begin{pmatrix} -1 \\ 1 \end{pmatrix}$.

Comparison between two directions



Which red line is better?

The best direction

Normalized data with d variables.

$$v_1, v_2, \dots, v_n \in \mathbb{R}^d$$

The best direction

Normalized data with d variables.

$$v_1, v_2, \ldots, v_n \in \mathbb{R}^d$$

The goal is to find the unit vector u that maximizes the variance in the direction of u i.e. the variance of

$$v_1 \cdot u, v_2 \cdot u, \ldots, v_n \cdot u$$

How can we find such u?

Answer: Look at the **covariance matrix** Σ.

Covariance matrix

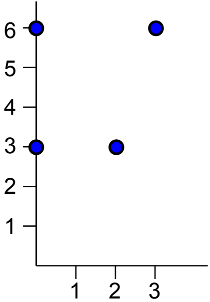
Let $X_1, X_2, \ldots, X_d$ be the variable vectors.

The covariance matrix is a $d \times d$ matrix defined by

$$\Sigma = \begin{bmatrix} \text{Cov}(X_1, X_1) & \text{Cov}(X_1, X_2) & \ldots & \text{Cov}(X_1, X_d) \\ \text{Cov}(X_2, X_1) & \text{Cov}(X_2, X_2) & \ldots & \text{Cov}(X_2, X_d) \\ \vdots & \vdots & \ddots & \vdots \\ \text{Cov}(X_d, X_1) & \text{Cov}(X_d, X_2) & \ldots & \text{Cov}(X_d, X_d) \end{bmatrix}$$

Example

$D = \{(0,3), (2,3), (3,6), (0,6)\}.$



Answer: $X_1 =$, $X_2 =$

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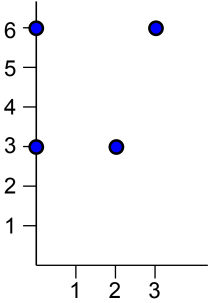
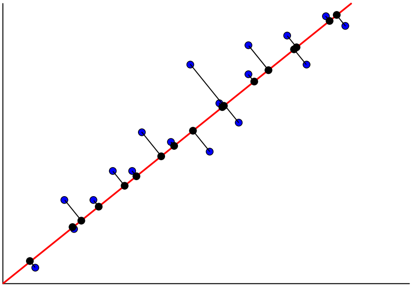


Answer: $X_1 =$, $X_2 =$

$$\Sigma = \begin{bmatrix} \mathrm{Var}(X_1) & \mathrm{Cov}(X_1, X_2) \\ \mathrm{Cov}(X_2, X_1) & \mathrm{Var}(X_2) \end{bmatrix} = \begin{bmatrix} 2.25 & 0.5 \\ 0.5 & 3 \end{bmatrix}.$$

Finding the best direction u



Data: $v_1, v_2, \ldots, v_n$

Projections on u: $(v_1 \cdot u, v_2 \cdot u, \ldots, v_n \cdot u)$

$$\text{Var}(v_1 \cdot u, \ldots, v_n \cdot u) = u^T \Sigma u.$$

Example

The data $D = \{(0,3),(2,3),(3,6),(0,6)\}$ has the covariance matrix

$$\Sigma = \begin{pmatrix} 2.25 & 0.5 \\ 0.5 & 3 \end{pmatrix}, \quad u = \frac{1}{\sqrt{5}}\begin{pmatrix} 1 \\ 2 \end{pmatrix}$$

The variance of the projections on u is

Spectral decomposition

Fact: Any symmetric matrix Σ can be decomposed as

$$\Sigma = \underbrace{\begin{pmatrix} \uparrow & \uparrow & & \uparrow \\ u_1 & u_2 & \dots & u_d \\ \downarrow & \downarrow & & \downarrow \end{pmatrix}}_{U^T} \underbrace{\begin{pmatrix} \lambda_1 & 0 & \dots & 0 \\ 0 & \lambda_2 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & \lambda_d \end{pmatrix}}_{\Lambda} \underbrace{\begin{pmatrix} \longleftarrow & u_1 & \longrightarrow \\ \longleftarrow & u_2 & \longrightarrow \\ & \vdots & \\ \longleftarrow & u_d & \longrightarrow \end{pmatrix}}_{U}$$

where

- $\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_d$ are the **eigenvalues**.
- $u_1, u_2, \ldots, u_d$ are the **eigenvectors** of length d.
- $u_1, u_2, \ldots, u_d$ are orthogonal unit vectors .

Eigenvectors

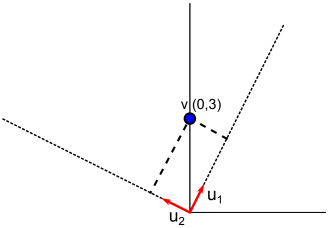
Fact: The eigenvectors $u_1, u_2, \ldots, u_d$ are:

- unit vectors
- perpendicular to each other.

Example

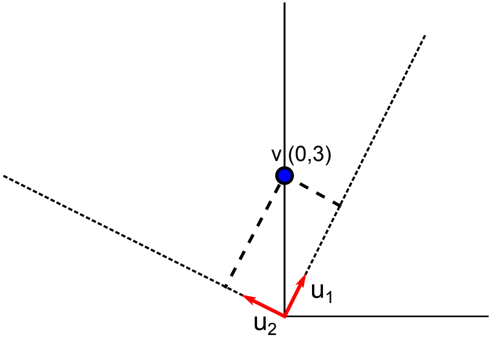
Compute Σu_1.

Example



$$\Sigma = \begin{pmatrix} 2.25 & 0.5 \\ 0.5 & 3 \end{pmatrix} = \begin{pmatrix} \frac{1}{\sqrt{5}} & -\frac{2}{\sqrt{5}} \\ \frac{2}{\sqrt{5}} & \frac{1}{\sqrt{5}} \end{pmatrix} \begin{pmatrix} 3.25 & 0 \\ 0 & 2 \end{pmatrix} \begin{pmatrix} \frac{1}{\sqrt{5}} & \frac{2}{\sqrt{5}} \\ -\frac{2}{\sqrt{5}} & \frac{1}{\sqrt{5}} \end{pmatrix}$$

- Eigenvalues:
- Eigenvectors:



The point $v = (0, 3)$ in the new axis is

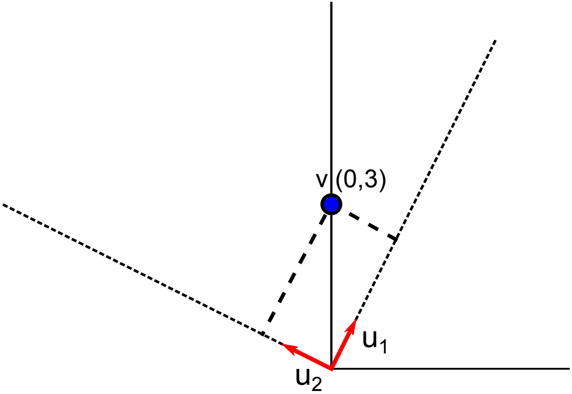
$$(v \cdot u_1, v \cdot u_2)$$

where

$$v \cdot u_1 =$$

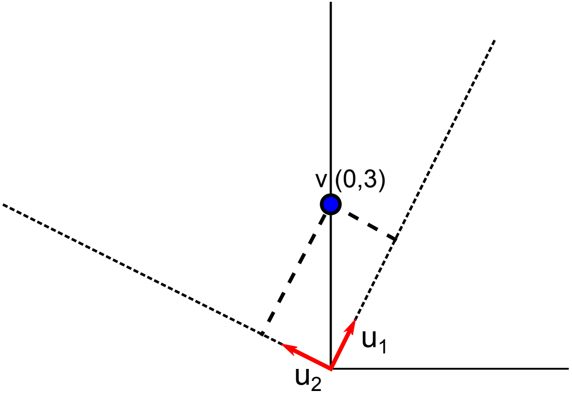
$$v \cdot u_2 =$$

Rotations preserve the length



Observation: $\|v\| = \|(v \cdot u_1, v \cdot u_2)\|$

Rotations preserve the length



Observation: $\|v\| = \|(v \cdot u_1, v \cdot u_2)\|$

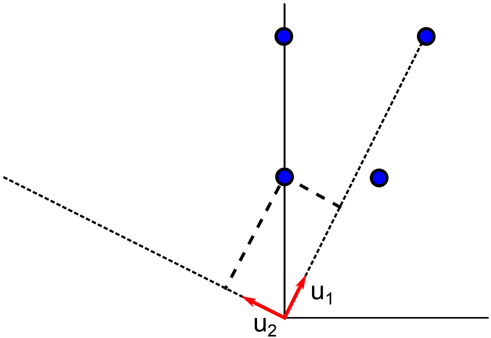
In higher dimension, $\|Uv\| = \|v\|$.

Finding the best direction u

$$\text{Var}(v_1 \cdot u, v_2 \cdot u, \ldots, v_n \cdot u)$$

Finding the best direction u

Example



- Variance $= 3.25$ in the direction of u_1.
- Variance $= 2$ in the direction of u_2.

Spectral decomposition

$$\Sigma = \begin{pmatrix} \uparrow & \uparrow & & \uparrow \\ u_1 & u_2 & \dots & u_d \\ \downarrow & \downarrow & & \downarrow \end{pmatrix} \begin{pmatrix} \lambda_1 & 0 & \dots & 0 \\ 0 & \lambda_2 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & \lambda_d \end{pmatrix} \begin{pmatrix} \longleftarrow & u_1 & \longrightarrow \\ \longleftarrow & u_2 & \longrightarrow \\ & \vdots & \\ \longleftarrow & u_d & \longrightarrow \end{pmatrix}$$

- The second best direction is u_2 with associated variance λ_2.
- The third best direction is u_3 with associated variance λ_3.
- and so on...

Principal component analysis

Let $u \in \mathbb{R}^d$ be a data point.

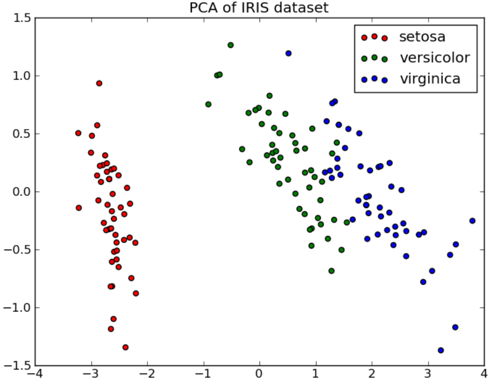
Principal axes ($k < d$):

$$u_1, u_2, \ldots, u_k$$

The PCA of u is

$$(u \cdot u_1, u \cdot u_2, \ldots, u \cdot u_k) \in \mathbb{R}^k.$$

PCA of iris flowers



$$\lambda_1 = 4.23, \quad \lambda_2 = 0.24$$
$$u_1 = (0.36, -0.08, 0.86, 0.36)$$
$$u_2 = (0.66, 0.73, -0.17, -0.07)$$

Three species of iris

- Setosa
- Versicolor
- Virginica

Four variables

- x_1: sepal length
- x_2: sepal width
- x_3: petal length
- x_4: petal width

Reconstruction

Eigenvectors: $u_1, u_2, \ldots, u_d$.

- k principal axes: $u_1, u_2, \ldots, u_k \in \mathbb{R}^d$.

- In these axes, the coordinate of the PCA of a point u is

$$(u \cdot u_1, u \cdot u_2, \ldots, u \cdot u_k) \in \mathbb{R}^k.$$

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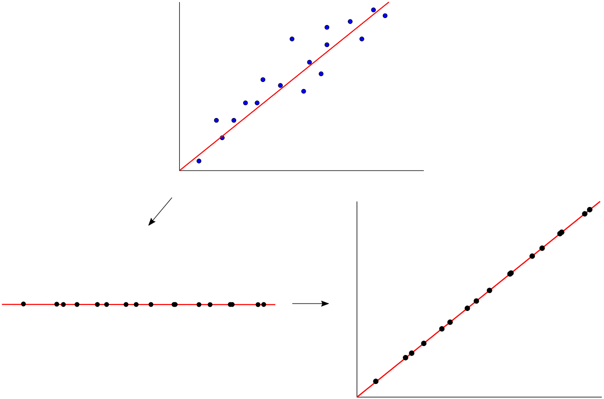
$$(u \cdot u_1, u \cdot u_2, \ldots, u \cdot u_k) \in \mathbb{R}^k.$$

  Reverse this point back to the original coordinate using

$$(u \cdot u_1)u_1 + (u \cdot u_2)u_2 + \ldots + (u \cdot u_k)u_k \in \mathbb{R}^d.$$

Reconstruction



The reconstructions are the black points on the red line. We see that there is some information loss in the process.

Reconstruction of MNIST

Reconstruct this original image x from its PCA projection to k dimensions.

$k = 200$ $\quad$ $k = 150$ $\quad$ $k = 100$ $\quad$ $k = 50$

Matrix as a transformation

$$M = \begin{pmatrix} 2.25 & 0.5 \\ 0.5 & 3 \end{pmatrix}$$

$$M \begin{pmatrix} 0 \\ 3 \end{pmatrix} = U^T \Lambda U \begin{pmatrix} 0 \\ 3 \end{pmatrix}$$