CS376 Machine Learning

Dimensionality Reduction & PCA

김기응

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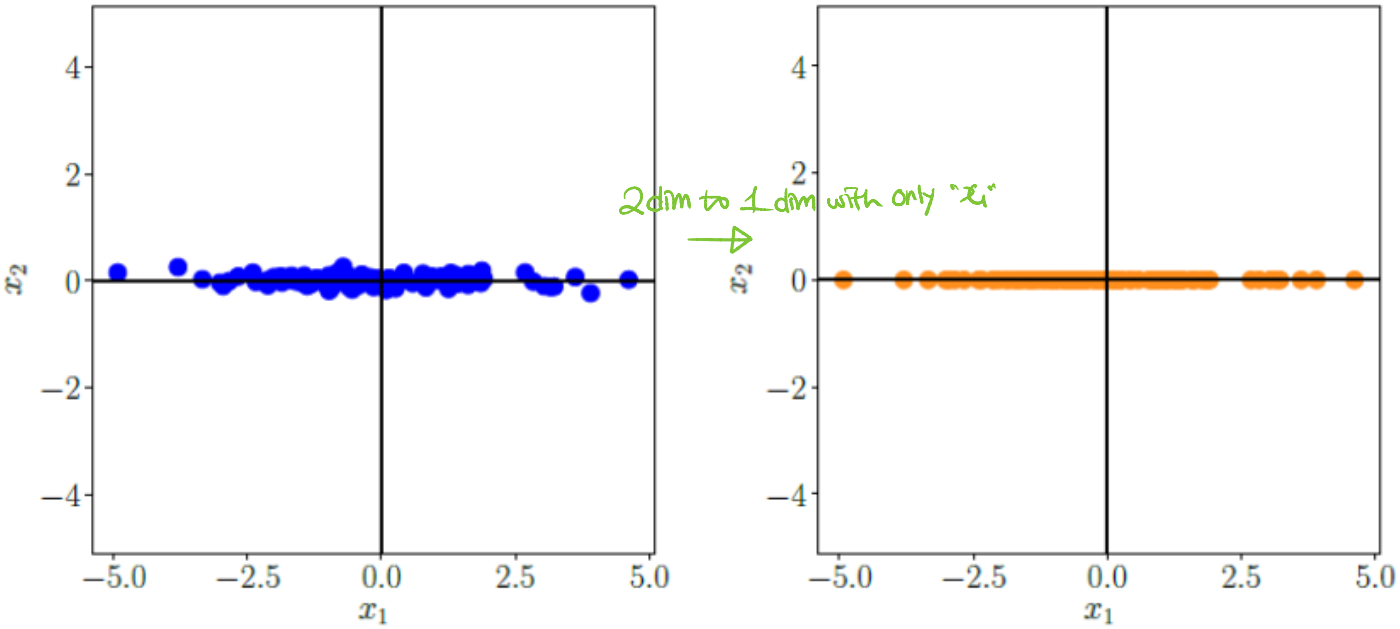
Motivation

Figure 10.1 Illustration: Dimensionality reduction. (a) The original dataset does not vary much along the x_2 direction. (b) The data from (a) can be represented using the x_1-coordinate alone with nearly no loss.



(a) Dataset with x_1 and x_2 coordinates.

(b) Compressed dataset where only the x_1 coordinate is relevant.

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Problem Setting

- Find projections $\tilde{x}_n$ of data points x_n that are as similar as possible, but with significantly lower dimensionality (intrinsic)
- $X = \{x_1 \dots x_N\}$, $x_n \in \mathbb{R}^D$ with mean 0. (important)
- Data covariance matrix

$$S = \frac{1}{N} \sum_{n=1}^{N} x_n x_n^T$$

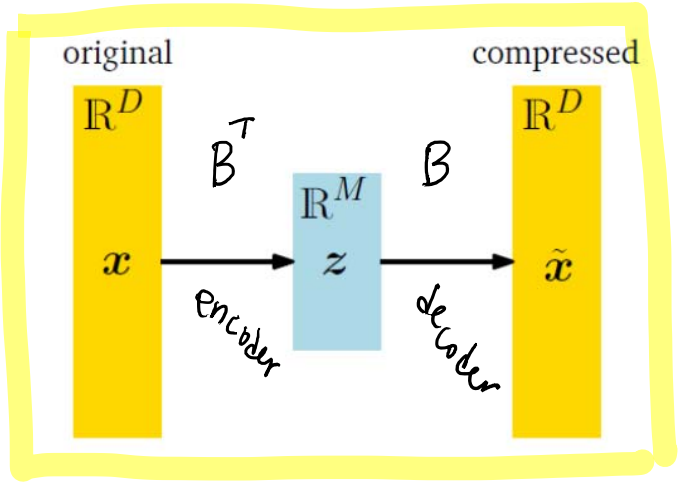
the columns $\boldsymbol{b}_1, \dots, \boldsymbol{b}_M$ of $\boldsymbol{B}$. Retaining most information after data compression is equivalent to capturing the largest amount of variance in the low-dimensional code (Hotelling, 1933).

- Find $z_n = B^T x_n \in \mathbb{R}^M$ $\quad B \triangleq [b_1 \dots b_M] \in \mathbb{R}^{D \times M}$

  $\{b_1 \dots b_M\}$ are orthonormal.

- $B^{-1} = B^T$, so $\tilde{x}_n = B z_n \in \mathbb{R}^D$

Figure 10.2 Graphical illustration of PCA. In PCA, we find a compressed version $\tilde{\boldsymbol{x}}$ of original data $\boldsymbol{x}$ that has an intrinsic lower-dimensional representation $\boldsymbol{z}$.



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$x \xrightarrow{B^T} z \xrightarrow{B} \tilde{x}$

$x \in \mathbb{R}^D$ $z \in \mathbb{R}^M$ $\tilde{x} \in \mathbb{R}^D$

10.2 Maximum Variance Perspective.

- Retain most informations after data compression 을 위해서는 capture the largest amount of variance in the low-dimensional code.

10.2.1 Direction with Maximal Variance

* single vector $b_1 \in \mathbb{R}^D$ that maximize the variance of projected data 구하기.

* maximize the variance of first coordinate z_1 of $z \in \mathbb{R}^M$

$\Rightarrow V_1 := \mathbb{V}[z_1] = \frac{1}{N}\sum_{n=1}^{N} z_{1n}^2$ $(z_n \in \mathbb{R}^M,\ x_n \in \mathbb{R}^D)$

z_1의 variance 구하는 식.

$z_{1n} = b_1^T x_n \rightarrow Z = B^T X$

$\therefore V_1 = \frac{1}{N}\sum_{n=1}^{N}(b_1^T x_n)^2 = \frac{1}{N}\sum_{n=1}^{N} b_1^T x_n x_n^T b_1 = b_1^T\left(\frac{1}{N}\sum_{n=1}^{N} x_n x_n^T\right) b_1 = b_1^T S b_1$ ∵ 이때 $\|b_1\|^2 = 1$

(data covariance matrix)

$\Rightarrow$ Optimization problem

$\max_{b_1} b_1^T S b_1 \quad s.t.\ \|b_1\|^2 = 1$

$\mathcal{L}(b_1, \lambda_1) = b_1^T S b_1 + \lambda_1(1 - b_1^T b_1)$

$\frac{d\mathcal{L}}{db_1} = 2b_1^T S - 2\lambda_1 b_1^T \qquad \frac{d\mathcal{L}}{d\lambda_1} = 1 - b_1^T b_1$

$\therefore Sb_1 = \lambda_1 b_1$ & $b_1^T b_1 = 1 \Leftrightarrow \lambda_1$: eigenvalue, b_1: eigenvector

$\Rightarrow V_1 = b_1^T S b_1 = \lambda_1 b_1^T b_1 = \lambda_1 \Leftrightarrow$ Variance 값 = eigenvalue 값

$\therefore$ variance 값이 클려면 eigenvalue 값 커야해.

이런식으로 $z \in \mathbb{R}^M$ 이내의 M-1 개의 큰 eigenvalue 값 뽑고, 해당 eigenvector로 $\underset{\sim}{B}$ 구성하기

$x \xrightarrow{B^T} z \xrightarrow{B} \tilde{x}$

$x \in \mathbb{R}^D$ $z \in \mathbb{R}^M$ $\tilde{x} \in \mathbb{R}^D$

10.2.2 M-dimensional subspace with Maximal Variance

※ Symmetric한 matrix ⟷ eigenvalue는 REAL

eigenvector는 orthonormal.

* M-1번째까지는 큰 eigenvalue를 구하고, M번째부터는 남는 애들 아무거나 값 쓰고 넘어

→ subtract the effect of the first m-1 principal components from the data, thereby trying to find principal components that compress the remaining information.

$\hat{X} := X - \sum_{i=1}^{m-1} b_i b_i^T X = X - B_{m-1} X$

⇒ $V_m = V[z_m] = \frac{1}{N}\sum_{n=1}^{N} z_{mn}^2 = \frac{1}{N}\sum_{n=1}^{N} (b_m^T \hat{x}_n)^2 = b_m^T \hat{S} b_m$.

⇒ 똑같이 optimize 하면. "b_m은 eigenvector of $\hat{S}$ with largest eigenvalue for $\hat{S}$"

그런데 사실 $S, \hat{S}$은 같은 sets of eigenvectors 가지고 있음.

↳ D개의 distinct한 eigenvector를 지님.

증명 만약 S의 m-1개의 eigenvector $b_1, b_2 \cdots b_{m-1}$ 찾고. b_i는 S의 eigenvector라면 $Sb_i = \lambda b_i$

$\hat{S} b_i = \frac{1}{N}\hat{X}\hat{X}^T b_i = \frac{1}{N}(X - B_{m-1}X)(X - B_{m-1}X)^T b_i = (S - SB_{m-1} - B_{m-1}S + B_{m-1}SB_{m-1}) b_i$

① $i \geq m$ $B_{m-1} b_i = 0$

$\hat{S} b_i = S b_i = \lambda b_i$

② $i < m$. $B_{m-1} b_i = b_i$

$\hat{S} b_i = 0 b_i = 0$ ⇒ eigenvalue = 0.

$b_1, b_2 \cdots b_{m-1}$: span NULL SPACE of $\hat{S}$

∴ every eigenvector of $S = \hat{S}$

S의 eigenvector이 (m-1)dim principal subspace라면 eigenvalue of $\hat{S} = 0$.

* M dimensional subspace에 project 되면, variance of data equals sum of the m개의 eigenvalues with high values : $V_M = \sum_{m=1}^{M} \lambda_m$

Maximum Variance Perspective

- First, we aim to maximize variance of the first coord z_1

$$V_1 \triangleq V[z_1] = \frac{1}{N}\sum_{n=1}^{N} z_{1n}^2$$

where $z_{1n} = b_1^T x_n$ (From $z = B^T x$)

$x \xrightarrow{B^T} z \xrightarrow{B} \tilde{x}$

- $V_1 = \frac{1}{N}\sum_{n=1}^{N} (b_1^T x_n)^2 = \frac{1}{N}\sum_{n=1}^{N} b_1^T x_n x_n^T b_1 = b_1^T \left(\frac{1}{N}\sum_{n=1}^{N} x_n x_n^T\right) b_1 = b_1^T S b_1$

S = "data covariance matrix"

- Thus, we need solve constrained optimization problem

$$\max_{b_1} b_1^T S b_1 \quad \text{subject to } \|b_1\|^2 = 1$$

$$\Leftrightarrow \mathcal{L}(b_1, \lambda) = b_1^T S b_1 + \lambda_1 (1 - b_1^T b_1)$$

$$\frac{\partial \mathcal{L}}{\partial b_1} = 2 b_1^T S - 2\lambda_1 b_1^T = 0 \qquad \frac{\partial \mathcal{L}}{\partial \lambda} = 1 - b_1^T b_1 = 0$$

$$\Leftrightarrow \begin{cases} S b_1 = \lambda_1 b_1 \\ b_1^T b_1 = 1 \end{cases} \Rightarrow$$

b_1 is an eigenvector of S.

λ_1 is the corresponding eigval.

$V_1 = b_1^T S b_1 = \lambda_1 b_1^T b_1 = \lambda_1 \Rightarrow$ Choose eigenvector with largest eigenvalue

"First principal component"

$\Rightarrow$ largest variance dir.

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Maximum Variance Perspective

- Assume we have found $m-1$ principal component. 지금까지는 이렇게 찾은 방식으로 eigenvalue 큰 거 골라.

  That is, we have found $b_1 \cdots b_{m-1}$, and find remaining PCs that compress remaining information → 마지막 m개는 남아있는 정보 가장 잘 압축할 수 있는 애로 고르기

  $$\hat{X} \triangleq X - \sum_{i=1}^{m-1} b_i b_i^T X \quad \text{where } X = [x_1 \cdots x_N] \in \mathbb{R}^{D \times N}$$

  원래 − 집어넣은 애 (!)

- $$\max V_m = V[z_m] = \frac{1}{N}\sum_{n=1}^{N} z_{mn}^2 = \frac{1}{N}\sum_{n=1}^{N} (b_m^T \hat{x}_n)^2 = b_m^T \hat{S} b_m$$

  Subject to $\|b_m\| = 1$ and $b_i^T b_m = 0$, $i = 1 \cdots m-1$

  $\Rightarrow$ b_m is the eigenvec with largest eigenval of $\hat{S}$

- This is also eigenvector of S

$$\hat{S} = \frac{1}{N}\sum_{n=1}^{N} \hat{x}_n \hat{x}_n^T = \frac{1}{N}\sum_{n=1}^{N} \left(x_n - \sum_{i=1}^{m-1} b_i b_i^T x_n\right)\left(x_n - \sum_{i=1}^{m-1} b_i b_i^T x_n\right)^T$$

$$= \frac{1}{N}\sum_{n=1}^{N}\Bigg[x_n x_n^T + \left(\sum_{i=1}^{m-1} b_i b_i^T\right) x_n x_n^T \left(\sum_{i=1}^{m-1} b_i b_i^T\right) - x_n x_n^T \left(\sum_{i=1}^{m-1} b_i b_i^T\right) - \left(\sum_{i=1}^{m-1} b_i b_i^T\right) x_n x_n^T \Bigg]$$

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Maximum Variance Perspective

- This is also eigenvector of S

$$\hat{S} = \frac{1}{N}\sum_{n=1}^{N} \hat{x}_n \hat{x}_n^T = \frac{1}{N}\sum_{n=1}^{N} \left(x_n - \sum_{i=1}^{m-1} b_i b_i^T x_n\right)\left(x_n - \sum_{i=1}^{m-1} b_i b_i^T x_n\right)^T$$

$$= \frac{1}{N}\sum_{n=1}^{N}\left[x_n x_n^T + \left(\sum_{i=1}^{m-1} b_i b_i^T\right) x_n x_n^T \left(\sum_{i=1}^{m-1} b_i b_i^T\right) - x_n x_n^T \left(\sum_{i=1}^{m-1} b_i b_i^T\right) - \left(\sum_{i=1}^{m-1} b_i b_i^T\right) x_n x_n^T\right]$$

$$\hat{S} b_m = \frac{1}{N}\sum_{n=1}^{N}\left[x_n x_n^T b_m + 0\right] - 0 = S b_m$$

last 0: proof

$$\frac{1}{N}\sum_{n=1}^{N}\sum_{i=1}^{m-1} b_i b_i^T x_n x_n^T b_m = \sum_{i=1}^{m-1} b_i b_i^T \underbrace{\left(\frac{1}{N}\sum_{n=1}^{N} x_n x_n^T\right)}_{S} b_m$$

$$= \sum_{i=1}^{m-1} b_i \lambda_i b_i^T b_m = 0$$

$$\therefore V_m = b_m^T \hat{S} b_m = b_m^T S b_m$$

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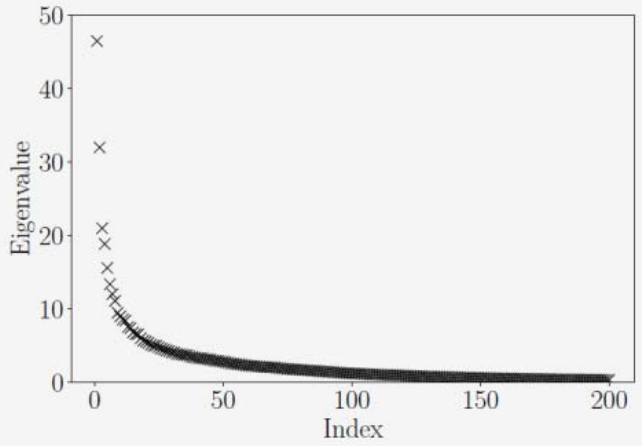
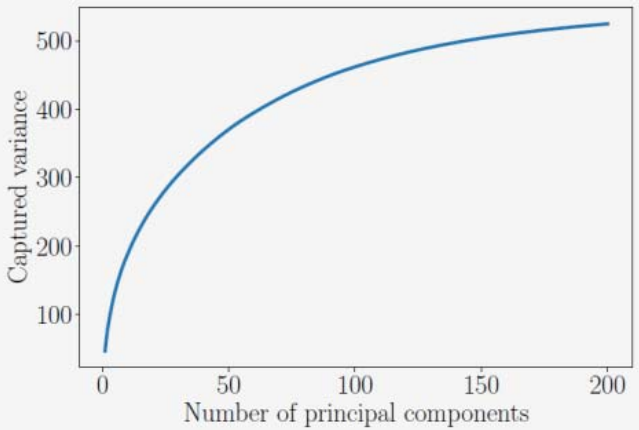
Maximum Variance Perspective



(a) Eigenvalues (sorted in descending order) of the data covariance matrix of all digits '8' in the MNIST training set.



(b) Variance captured by the principal components.

- The amount of variance captured by PCA using M PCs

$$V_M = \sum_{m=1}^{M} \lambda_m$$

The amount of variance lost by PCA

$$J_M = \sum_{j=M+1}^{D} \lambda_j = V_D - V_M$$

relative measure: $\frac{V_M}{V_D}$, $1 - \frac{V_M}{V_D}$

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Projection Perspective

- PCA as an algorithm that directly minimizes avg reconstruction error ($\|x_n - \tilde{x}_n\|$)
- Assume ordered orthonormal basis $B = (b_1 \cdots b_D)$, ie $b_i^T b_j = 1$ iff $i = j$ and 0 otherwise
- Any $x \in \mathbb{R}^D$, $x = \sum_{d=1}^{D} \zeta_d b_d = \sum_{m=1}^{M} \zeta_m b_m + \sum_{j=M+1}^{D} \zeta_j b_j$

$$\tilde{x} = \sum_{m=1}^{M} z_m b_m \in U \subseteq \mathbb{R}^D \text{ with } \dim(U) = M$$

RM z_m and ζ_m are not identical? identical? $\in \mathbb{R}$!

Projection Perspective

a $\min \quad J_M \triangleq \frac{1}{N} \| x_n - \tilde{x}_n \|^2$ ($\tilde{x}_n = B^T z$)

$z_1 \cdots z_n$

$b_1 \cdots b_m$

Finding $z_1 \cdots z_n$

e $\frac{\partial J_M}{\partial z_{in}} = \frac{\partial J_M}{\partial \tilde{x}_n} \frac{\partial \tilde{x}_n}{\partial z_{in}}$,

$$\begin{cases} \frac{\partial J_M}{\partial \tilde{x}_n} = -\frac{2}{N}(x_n - \tilde{x}_n)^T \in \mathbb{R}^{1 \times D} \\ \frac{\partial \tilde{x}_n}{\partial z_{in}} = \frac{\partial}{\partial z_{in}} \left(\sum_{m=1}^{M} z_{mn} b_m \right) = b_i \end{cases}$$

$$= -\frac{2}{N}(x_n - \tilde{x}_n)^T b_i = -\frac{2}{N}\left(x_n - \sum_{m=1}^{M} z_{mn} b_m\right)^T b_i$$

나머지 같은 orthonormal이니 없애도

$$= -\frac{2}{N}(x_n^T b_i - z_{in} b_i^T b_i) = -\frac{2}{N}(x_n^T b_i - z_{in}) = 0$$

$\therefore z_{in} = x_n^T b_i = b_i^T x_n$ (z_{in} is the coordinate of ortho. projection of x_n onto b_i)

Note ① ξ_m and z_m are identical for $m = 1 \cdots M$

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Low-Rank Approximation Perspective

finding $b_1 \cdots b_M$

② $z_n = B^T x_n$, $\tilde{x}_n = B z_n$ (D, D×M, M)

$B = [b_1 \cdots b_M] \in \mathbb{R}^{D \times M}$

D → M → D

$$\tilde{x}_n = \sum_{m=1}^{M} z_{mn} b_m = \sum_{m=1}^{M} (x_n^T b_m) b_m = \left(\sum_{m=1}^{M} b_m b_m^T \right) x_n$$

$$x_n = \sum_{d=1}^{D} z_{dn} b_d = \sum_{d=1}^{D} (x_n^T b_d) b_d = \left(\sum_{d=1}^{D} b_d b_d^T \right) x_n$$

$$= \left(\sum_{m=1}^{M} b_m b_m^T \right) x_n + \left(\sum_{j=M+1}^{D} b_j b_j^T \right) x_n$$

$$x_n - \tilde{x}_n = \left(\sum_{j=M+1}^{D} b_j b_j^T \right) x_n = \sum_{j=M+1}^{D} (x_n^T b_j) b_j$$

Low rank Approx. View

$$\tilde{x}_n = \left(\sum_{m=1}^{M} b_m b_m^T \right) x_n = BB^T x_n$$ (BB^T is of rank $\leq M$)

$$J_M = \frac{1}{N} \sum_{n=1}^{N} \| x_n - \tilde{x}_n \|^2 = \frac{1}{N} \sum_{n=1}^{N} \| x_n - BB^T x_n \|^2 = \frac{1}{N} \sum_{n=1}^{N} \| (I - BB^T) x_n \|^2$$

(Try to find the best rank-M approximation of BB^T to I)

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Low-Rank Approximation Perspective

$$J_M = \frac{1}{N}\sum_{n=1}^{N} \|x_n - \tilde{x}_n\|^2 = \frac{1}{N}\sum_{n=1}^{N} \left\| \sum_{j=M+1}^{D} (b_j^T x_n) b_j \right\|^2 = \frac{1}{N}\sum_{n=1}^{N}\sum_{j=M+1}^{D} (b_j^T x_n)^2$$

$$= \frac{1}{N}\sum_{n=1}^{N}\sum_{j=M+1}^{D} b_j^T x_n x_n^T b_j = \sum_{j=M+1}^{D} b_j^T \left(\frac{1}{N}\sum_{n=1}^{N} x_n x_n^T\right) b_j = \sum_{j=M+1}^{D} b_j^T S b_j$$

$$= \sum_{j=M+1}^{D} \mathrm{tr}(b_j^T S b_j) = \sum_{j=M+1}^{D} \mathrm{tr}(b_j b_j^T S) = \mathrm{tr}\left(\left(\sum_{j=M+1}^{D} b_j b_j^T\right) S\right)$$

$$= \sum_{j=M+1}^{D} \lambda_j$$

(minimize the variance of data when projected on to the subspace we ignore)

= (select $(D-M)$ eigenvectors with smallest eigvalues)

= (select D eigenvectors with largest eigvalues)

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PCA Illustration

Example 10.3 (MNIST Digits Embedding)

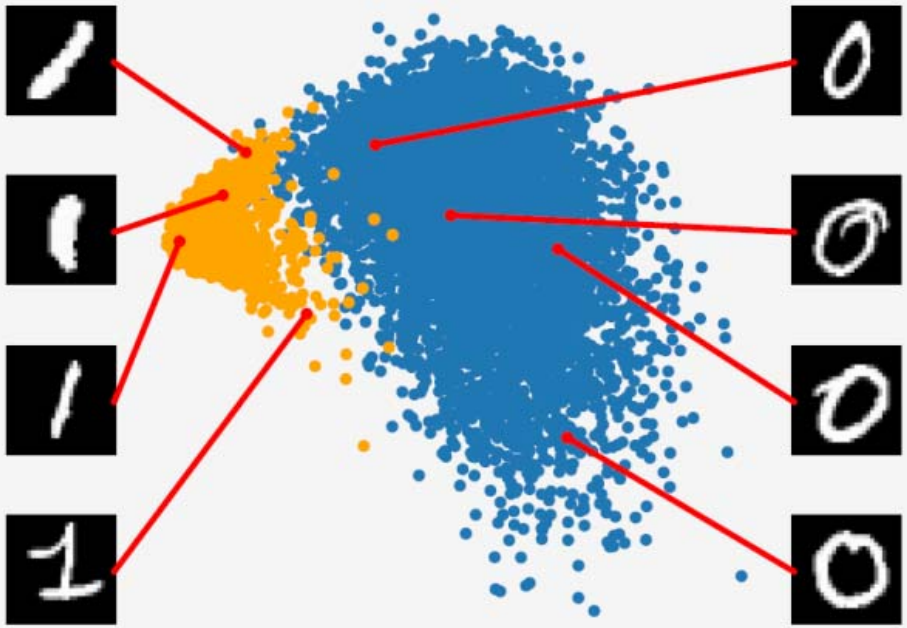

Figure 10.10 Embedding of MNIST digits 0 (blue) and 1 (orange) in a two-dimensional principal subspace using PCA. Four embeddings of the digits '0' and '1' in the principal subspace are highlighted in red with their corresponding original digit.