Machine Learning Exercise Sheet 11

Dimensionality Reduction & Matrix Factorization

Homework

PCA & SVD

Problem 1: Use the SVD shown below. Suppose a new user Leslie assigns rating 3 to Alien and

	Matrix	Alien	Star Wars	Casablanca	Titanic
Joe	1	1	1	0	0
Jim	3	3	3	0	0
John	4	4	4	0	0
Jack	5	5	5	0	0
Jill	0	0	0	4	4
Jenny	0	0	0	5	5
Jane	0	0	0	2	2
Leslie	0	3	0	0	4

$\tilde{M} = M \cdot V^T = M \cdot U \Sigma$

Figure 11.6: Ratings of movies by users

$$\underbrace{\begin{bmatrix} 1 & 1 & 1 & 0 & 0 \\ 3 & 3 & 3 & 0 & 0 \\ 4 & 4 & 4 & 0 & 0 \\ 5 & 5 & 5 & 0 & 0 \\ 0 & 0 & 0 & 4 & 4 \\ 0 & 0 & 0 & 5 & 5 \\ 0 & 0 & 0 & 2 & 2 \end{bmatrix}}_{M} = \underbrace{\begin{bmatrix} .14 & 0 \\ .42 & 0 \\ .56 & 0 \\ .70 & 0 \\ 0 & .60 \\ 0 & .75 \\ 0 & .30 \end{bmatrix}}_{U} \underbrace{\begin{bmatrix} 12.4 & 0 \\ 0 & 9.5 \end{bmatrix}}_{\Sigma} \underbrace{\begin{bmatrix} .58 & .58 & .58 & 0 & 0 \\ 0 & 0 & 0 & .71 & .71 \end{bmatrix}}_{V^{\mathrm{T}}}$$

rating 4 to Titanic, giving us a representation of Leslie in the 'original space' of $[0, 3, 0, 0, 4]$. Find the representation of Leslie in concept space. What does that representation predict about how well Leslie would like the other movies appearing in our example data?

Problem 2: Consider the latent space distribution

$$p(\boldsymbol{z}) = \mathcal{N}(\boldsymbol{z}|\boldsymbol{0}, \boldsymbol{I})$$

and a conditional distribution for the observed variable $\boldsymbol{x} \in \mathbb{R}^d$,

$$p(\boldsymbol{x}|\boldsymbol{z}) = \mathcal{N}(\boldsymbol{x}|\boldsymbol{W}\boldsymbol{z} + \boldsymbol{\mu}, \boldsymbol{\Phi})$$

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where $\boldsymbol{\Phi}$ is an arbitrary symmetric, positive-definite noise covariance variable. Now suppose that we make a nonsingular linear transformation of the data variables $\boldsymbol{y} = \boldsymbol{A}\boldsymbol{x}$ where $\boldsymbol{A}$ is a non-singular $d \times d$ matrix. If $\boldsymbol{\mu}_{ML}$, $\boldsymbol{W}_{ML}$, and $\boldsymbol{\Phi}_{ML}$ represent the maximum likelihood solution corresponding to the original untransformed data, show that $\boldsymbol{A}\boldsymbol{\mu}_{ML}$, $\boldsymbol{A}\boldsymbol{W}_{ML}$, and $\boldsymbol{A}\boldsymbol{\Phi}_{ML}\boldsymbol{A}^T$ will represent the corresponding maximum likelihood solution for the transformed data set. Finally, show that the form of the model is preserved if $\boldsymbol{A}$ is orthogonal and $\boldsymbol{\Phi}$ is proportional to the unit matrix so $\boldsymbol{\Phi} = \sigma^2\boldsymbol{I}$ (i.e. probabilistic PCA). The transformed $\boldsymbol{\Phi}$ matrix remains proportional to the unit matrix, and hence probabilistic PCA is covariant under a rotation of the axes of data space, as is the case for conventional PCA.

Problem 3: Let the matrix $\boldsymbol{X} \in \mathbb{R}^{N\times D}$ represent N data points of dimension $D = 10$ (samples stored as rows). We applied PCA to $\boldsymbol{X}$. By using the $K = 5$ top principal components, we transformed/projected $\boldsymbol{X}$ into $\tilde{\boldsymbol{X}} \in \mathbb{R}^{N\times K}$. We computed that $\tilde{\boldsymbol{X}}$ preserves 70% of the variance of the original data $\boldsymbol{X}$.

Suppose now we apply PCA on the following matrices:

a) $\boldsymbol{Y}_1 = \boldsymbol{X}\boldsymbol{S}$ where $\boldsymbol{S} = \lambda\boldsymbol{I}$, with $\lambda \in \mathbb{R}$ and $\boldsymbol{I} \in \mathbb{R}^{D\times D}$ is the identity matrix

b) $\boldsymbol{Y}_2 = \boldsymbol{X}\boldsymbol{R}$ where $\boldsymbol{R} \in \mathbb{R}^{D\times D}$ and $\boldsymbol{R}\boldsymbol{R}^T = \boldsymbol{I}$

c) $\boldsymbol{Y}_3 = \boldsymbol{X}\boldsymbol{P}$ where $\boldsymbol{P} = \operatorname{diag}(+5, -5, \dots, +5, -5)$ is a $D \times D$ diagonal matrix

d) $\boldsymbol{Y}_4 = \boldsymbol{X}\boldsymbol{Q}$ where $\boldsymbol{Q} = \operatorname{diag}(1, 2, 3, \dots, D-1, D)$ is a $D \times D$ diagonal matrix

e) $\boldsymbol{Y}_5 = \boldsymbol{X} + \boldsymbol{1}_N\boldsymbol{\mu}^T$ where $\boldsymbol{\mu} \in \mathbb{R}^D$ and $\boldsymbol{1}_N$ is an N-dimensional column vector of all ones

f) $\boldsymbol{Y}_6 = \boldsymbol{X}\boldsymbol{A}$ where $\boldsymbol{A} \in \mathbb{R}^{D\times D}$ and $\operatorname{rank}(\boldsymbol{A}) = 5$

and obtain the projected data $\tilde{\boldsymbol{Y}}_1, \dots \tilde{\boldsymbol{Y}}_6 \in \mathbb{R}^{N\times K}$ using the principal components corresponding to the top $K = 5$ largest eigenvalues of the respective $\boldsymbol{Y}_i$.

What fraction of variance of each $\boldsymbol{Y}_i$ will be preserved by each respective $\tilde{\boldsymbol{Y}}_i$? *Justify your answer.*

The answer "cannot tell without additional information" is also valid if you provide a justification.

Problem 4: You are given $N = 4$ data points: $\{\boldsymbol{x}_i\}_{i=1}^4$, $\boldsymbol{x}_i \in \mathbb{R}^3$, represented with the matrix $\boldsymbol{X} \in \mathbb{R}^{4\times 3}$.

$$\boldsymbol{X} = \begin{bmatrix} 4 & 3 & 2 \\ 2 & 1 & -2 \\ 4 & -1 & 2 \\ -2 & 1 & 2 \end{bmatrix}$$

Hint: In this task the results of all (final and intermediate) computations happen to be integers.

a) Perform principal component analysis (PCA) of the data $\boldsymbol{X}$, i.e. find the principal components and their associated variances in the transformed coordinate system. Show your work.

b) Project the data to two dimensions, i.e. write down the transformed data matrix $\boldsymbol{Y} \in \mathbb{R}^{4\times 2}$ using the top-2 principal components you computed in (a). What fraction of variance of $\boldsymbol{X}$ is preserved by $\boldsymbol{Y}$?

c) Let $\boldsymbol{x}_5 \in \mathbb{R}^3$ be a new data point. Specify the vector $\boldsymbol{x}_5$ such that performing PCA on the data including the new data point $\{\boldsymbol{x}_i\}_{i=1}^5$ leads to exactly the same principal components as in (a).

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Problem 5: Load the notebook `exercise_11_notebook.ipynb` from Piazza. Fill in the missing code and run the notebook. Convert the evaluated notebook to pdf and add it to the printout of your homework.

In-class Exercises

Probabilistic PCA

Problem 6: For pPCA, we consider the latent space distribution

$$p(\boldsymbol{z}) = \mathcal{N}(\boldsymbol{z}|\boldsymbol{0}, \boldsymbol{I})$$

and a conditional distribution for the observed variable $\boldsymbol{x} \in \mathbb{R}^d$,

$$p(\boldsymbol{x}|\boldsymbol{z}) = \mathcal{N}(\boldsymbol{x}|\boldsymbol{W}\boldsymbol{z} + \boldsymbol{\mu}, \sigma^2\boldsymbol{I})$$

a) Verify that the covariance of the marginal distribution $p(\boldsymbol{x}) = \mathcal{N}(\boldsymbol{x}|\boldsymbol{\mu}, \boldsymbol{C})$ is given by $\boldsymbol{C} = \boldsymbol{W}\boldsymbol{W}^T + \sigma^2\boldsymbol{I}$. What is the interpretation of this result?

b) Verify that the model is unidentifiable, i.e. that the matrix $\boldsymbol{W}$ is only defined up to a rotation $\boldsymbol{R}$! What is the interpretation of this result?

c) Derive an expression for the posterior of the latent variables $p(\boldsymbol{z}|\boldsymbol{x})$!