

3.  $\|x_i - x_j\|_2 = \|z_i - z_j\|_2$ . Lets take a look at  $\|z_i - z_j\|_2$ :

$$\begin{aligned}\|z_i - z_j\| &= \|U^T(x_i - \mu_x) - U^T(x_j - \mu_x)\| \\ &= \|U^T x_i - U^T \mu_x - U^T x_j + U^T \mu_x\| \\ &= \|U^T\| \cdot \|x_i - x_j\| = \|x_i - x_j\|\end{aligned}$$

2

-2

### 1.2.2

Let  $U_d \in \mathbb{R}^{D \times d}$  be a fully ranked matrix (with  $d \leq D$ ). Since  $U$  is fully ranked, we can use SVD and denote  $U_d = U' \Sigma' V'^T$  where  $U' \in \mathbb{R}^{D \times D}$ ,  $\Sigma' \in \mathbb{R}^{D \times d}$ ,  $V' \in \mathbb{R}^{d \times d}$ . We will notice that  $V'^T V' = I_d$ , and that  $\Sigma'^{-1}$  exists (every diagonal matrix has an invert)

We will denote  $M = V' \Sigma'^{-1}$ ,  $O = U_d M$  and we will take a look at  $O^T O$ :

$$\begin{aligned}O^T O &= M^T U_d^T U_d M \\ &= (\Sigma'^{-1})^T V'^T V' \Sigma'^T U'^T U' \Sigma' V'^T V' \Sigma'^{-1} = \\ &=^* (\Sigma'^{-1})^T I_d \Sigma'^T I_d \Sigma' I_d \Sigma'^{-1} = I_d\end{aligned}$$

-1

(\*)  $V'^T V' = I_d$ ,  $U'^T U' = I_D$

$\Sigma_x$  is not square

You should have used the compact SVD instead.

### 1.2.6

$X \in \mathbb{R}^{D \times N}$  where  $D > N$ .

A tight upper bound to the number of non zero eigenvalues would be  $N$ .

Lets take an example  $I_N \in \mathbb{R}^{D \times N} =$

$$\begin{pmatrix} 1 & 0 & \dots & 0 \\ 0 & 1 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & \dots & \dots & 1 \\ 0 & \dots & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots \\ 0 & \dots & \dots & 0 \end{pmatrix}$$

In  $I_D$ , there are  $N$  eigenvectors (each one of the columns is an eigenvector)

Now, Since the  $\text{Rank}(X) \leq \min(N, D) = N$ , it means that  $X$  can be spread with  $N$  independent vectors, so there can not be more than  $N$  eigenvalues greater than 0.

What about the second part?

-2

### 1.2.7

Let  $A \in \mathbb{R}^{D \times N}$  and we have the following minimization problem:

$$\begin{cases} \min_{M \in \mathbb{R}^{D \times N}} \|A - M\|_F^2 \\ \text{s.t. } \text{rank}(M) \leq d \end{cases}$$

*A is not square*

We will notice, that because  $\text{rank}(M) = d$  then  $d \leq \min(D, N)$  and therefore we have two matrices  $B \in \mathbb{R}^{D \times d}$ ,  $C \in \mathbb{R}^{d \times N}$  with ranks  $d$  such that  $M = BC$ . We also saw in class the the solution of this minimization problem is  $\tilde{C} = B_d^T A$  where  $B_d$  are eigenvectors of A, and we have only  $d$  of them and all the rest of B's columns are 0.

We also know that every matrix  $M \in \mathbb{R}^{D \times N}$  can be expressed as  $M = U \Sigma V^T$ . Because  $M$ 's rank is  $d$ , then we will have the truncated version  $M = U_d \Sigma_d V_d^T$  where again  $U_d$  are matrix with  $d$  eigenvectors of A,  $\Sigma_d$  has  $d$  eigenvalues along the diagonal and the rest of the diagonal is 0 (if not truncated) and  $V_d^T$  is a row-vector matrix where we have again  $d$  vecotrs which are non-zero.

4

*2*

*+2*

To be honest, I tried and tried, and didn't figure out how to combine both these points into a final solution. I tried to transform  $B_d C_d$  into a representation of  $U_d \Sigma_d V_d^T$  but unfortunately couldn't find the right way.

Prove:  $k(x_i, x_j) = (1 + x_i^T x_j)^2$  is a kernel function.

Lets write :

$$\phi(x) = 1 + 2x_i^T x_j + x_i^2 \begin{bmatrix} 1 \\ \sqrt{2}x \\ x^2 \end{bmatrix}$$

Now, lets show that  $k(x_i, x_j) = \langle \phi(x_i), \phi(x_j) \rangle$

$$\begin{aligned} k(x_i, x_j) &= (1 + x_i^T x_j)^2 \\ &= (1 + x_i^T x_j)(1 + x_i^T x_j) \\ &= 1 + 2x_i^T x_j + (x_i^T x_j)^2 \end{aligned}$$

*-2*

-2

$$\begin{aligned}
 &= (1 + x_i^T x_j)(1 + x_i^T x_j) \\
 &= 1 + 2x_i^T x_j + (x_i^T x_j)^2 \\
 &= \left\langle \begin{bmatrix} 1 \\ \sqrt{2}x_i \\ x_i^2 \end{bmatrix}, \begin{bmatrix} 1 \\ \sqrt{2}x_j \\ x_j^2 \end{bmatrix} \right\rangle \\
 &= \langle \phi(x_i), \phi(x_j) \rangle
 \end{aligned}$$

### 2.1.7 OOS extension

Let  $K_x$  be the kernel matrix obtained from the training set  $\chi = \{x_i \in \mathbb{R}^D\}_{i=1}^N$ , let  $Z \in \mathbb{R}^{d \times N}$  be the low-dimensional representation obtained by applying KPCA, that is:  $Z = \Sigma_d V_d^T$  and let  $X^* \in \mathbb{R}^{D \times N}$  be a set of new unseen data-points.

We will denote  $\Phi^* = \phi(X^*)$  and  $K_x^* = \Phi^{*T} \Phi$ .

Then from what we learned in the lecture, we can represent the KPCA of the OOS extension applied on  $X^*$  as:

$$Z^* = \Sigma_d^{-1} V_d^T \Phi^{*T} \Phi^* \neq \Sigma_d^{-1} V_d^T \tilde{K}_x^*$$

Since  $\tilde{K}_x^* = J(k_x - \frac{1}{N} K_x 1_N)$

$\mathbb{R}^{N \times N^*} \neq \mathbb{R}^{N^* \times N}$

$$Z^* = \Sigma_d^{-1} V_d^T \tilde{K}_x^* \neq \Sigma_d^{-1} V_d^T J(k_x - \frac{1}{N} K_x 1_N)$$

-2

```

4 class PCA:
5     def __init__(self, d):
6         self.d = d
7         self.vMean = None
8         self.mUd = None
9         self.vSig = None
10
11     def Fit(self, mX):
12         ...
13         Learns model's parameters
14         Args:
15             mX - Input training data, mX.shape = (D, N)
16         Output:
17             self
18         ...
19
20         svds_values = svds(mX, self.d)
21         eigen_vectors, eigen_values = svds_values[0], svds_values[1]
22
23         idx = eigen_values.argsort()[::-1]
24         self.mUd = eigen_vectors[:,idx]
25         self.vSig = eigen_values[idx]
26         self.vMean = svds_values[2]
27

```

-2

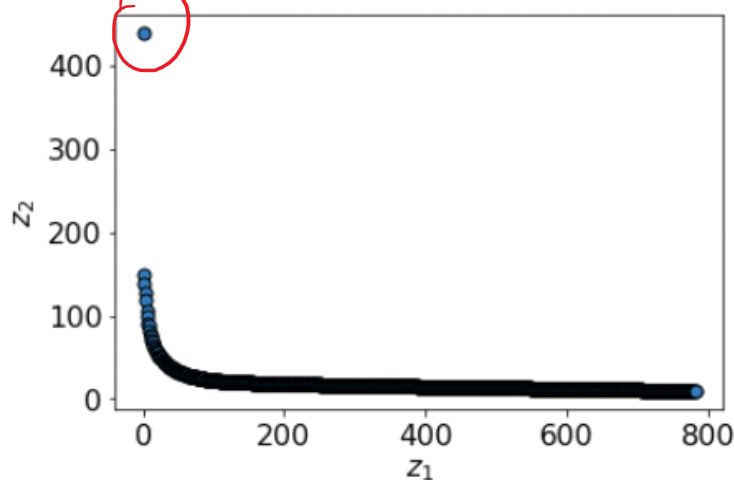
1. You need to remove the mean first
2. What?!

## 2. What?!

```

1  _, eigenvalues, _ = svds(mX, mX.shape[0] - 1)
2
3  eigenvalues = np.flip(eigenvalues) #sort from higher to lower
4
5  plt.scatter(range(len(eigenvalues)), eigenvalues, s=50, edgecolor='k')
6  plt.xlabel('$z_1$')
7  plt.ylabel('$z_2$')
8  plt.show()

```



need to remove the mean

```

3  class KPCA:
4      def __init__(self, d, k):
5          self.d = d
6          self.k = k
7          pass
8
9      def Fit(self, mX):
10         ...
11         Learns model's parameters
12         Args:
13             mX - Input training data, mX.shape = (D, N)
14         Output:
15             self
16         ...
17
18         N = mX.shape[1]
19         kernel = self.k(mX, mX)
20         J = np.identity(N) - np.ones((N, N)) / N
21         self.mX = mX
22         self.K = kernel @ J
23
24         svds_values = svds(self.K, self.d)
25         eigen_vectors, eigen_values = svds_values[0], svds_values[1]
26
27         idx = eigen_values.argsort()[::-1]
28         self.mVd = eigen_vectors[:,idx]
29         self.vSig = np.sqrt(eigen_values[idx])
30
31     def Encode(self, mXstar):
32         ...
33         Apply (out of sample) encoding
34         Args:
35             mXstar - Input data, mX.shape = (D, Nstar)
36         Output:
37             mZ - Low-dimensional representation (embeddings), mZ.shape = (d, Nstar)
38         ...
39         return mZ

```

Handwritten notes:

- $\tilde{K} = J K J$
- $\tilde{K} = U \Sigma^2 U^T$
- ③

```

36     Output:
37     ... mZ      - Low-dimensional representation (embeddings), mZ.shape = (d, Nstar)
38
39     return np.linalg.inv(np.diag(self.vSig)) @ self.mVd.T @ self.k(self.mX, mXstar)
40

```

```

1  from scipy.spatial.distance import cdist
2  def mat_mul_kernel(mX1, mX2):
3      return mX1.T @ mX2
4
5  def polynomial_kernel(mX1, mX2, p=2):
6      return (1 + mX1.T @ mX2) ** p
7
8  def gaus_kernel(mX1, mX2):
9      distances_matrix = cdist(mX1.T, mX2.T)
10     sigma = np.mean(distances_matrix)
11     return np.exp(-distances_matrix / (2 * sigma * sigma))

```

1. sigma must be a fixed value
2. dist\_mat \*\* 2