Section 09: PCA and SVD

1. Using the Eigenbasis

It's a very useful fact that for any symmetric n×n matrix A you can find a set of eigenvectors u_1, ..., u_n for A such that:

- $\|u_i\|_2 = 1$
- $u_i^T u_j = 0, \forall i \neq j$
- $u_1, \ldots, u_n$ form a basis of $\mathbb{R}^n$

One of the reasons this fact is useful is that facts about these matrices are easier to prove if you think about the vectors in terms of their "eigenbasis" components, instead of their components in the standard basis. As a trivial example, we'll show that you can calculate Ax for a vector x without having to do the matrix multiplication.

(a) Consider the matrix $A = \begin{bmatrix} 4 & -1 \\ -1 & 4 \end{bmatrix}$. Verify that $u_1 = \begin{bmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \end{bmatrix}$ and $u_2 = \begin{bmatrix} -1/\sqrt{2} \\ 1/\sqrt{2} \end{bmatrix}$ are eigenvectors and meet the definitions. Find the eigenvalues associated with u_1 and u_2

(b) since $\{u_1, u_2\}$ are a basis, we can write any vector as a linear combination of them. Write $x = \begin{bmatrix} -1/\sqrt{2} \\ 3/\sqrt{2} \end{bmatrix}$ in this basis.

(c) Based on the eigenvectors and eigenvalues your found in part a, diagonalize A, i.e, find matrix U and D such that $UDU^T = A$ where all entries of D are 0 except for the ones on the diagonal.

(d) Use the decomposition and the eigenvalues you calculated to calculate Ax wihtout doing matrix-vector multiplication.

This method of calculating a matrix vector product won't actually be more computationally efficient – but it's what's "really" happening when you do the multiplication, so this will be useful intuition under certain circumstances. Expressing vectors in an eigenbasis is also a useful proof technique, as we'll see in some later problems.

2. Singular Value Decomposition - Proofs

Recall that if we have a symmetric, square matrix A $\in \mathbb{R}^{n\times n}$, we can eigen-decompose it in the form of $A = USU^T$, where the columns of U are eigenvectors of A with lengths of 1, and the diagonal of S is the list of eigenvalues corresponding to those eigenvectors.
Now, for a more general case, where A is a data matrix with the dimension of $\mathbb{R}^{n\times d}$, there is still a way to decompose it: $A = USV^T$, where $U \in \mathbb{R}^{n\times n}$, S is a rectangular diagonal matrix and $S \in \mathbb{R}^{n\times d}$, and $V \in \mathbb{R}^{d\times d}$.
It is called Singular Value Decomposition (SVD).

(a) Let A have SVD USV^T. Show AA^T has the columns of U as eigenvectors with associated eigenvalues S^2.

(b) Let A have SVD USV^T. Show $A^T A$ has the columns of V as eigenvectors with associated eigenvalues S^2.

(c) For the matrix A, suppose we are given that $AA^T = US^2U^T$ and $A^TA = VS^2V^T$. Show that $A = USV^T$. I.e., show that for any vector $x \in \mathbb{R}^d$, we have $Ax = USV^Tx$

3. Principal Component

Consider the following dataset, which is represented as three points in $\mathbb{R}^2$. Note that in this problem we will **not** demean the dataset.

$$\begin{bmatrix} 1 & 2 \\ 1.5 & 3 \\ 6 & 12 \end{bmatrix}$$

(a) What is the first principal component vector, v_1?

(b) What is the second principal component, v_2?

(c) If we use only the first principal component to compress the dataset, what will the representation of each point be?

(d) Will this representation be lossy, or perfectly preserve the dataset?

Answer the same questions for the following, slightly larger dataset:

$$\begin{bmatrix} 1 & 1 \\ 1.5 & 1.5 \\ -2 & 2 \\ 4 & -4 \\ 6 & -6 \\ 2 & 2 \end{bmatrix}$$

(a) What is the first principal component vector, v_1?

(b) What is the second principal component, v_2?

(c) If we use only the first principal component to compress the dataset, what will the representation of each point be?

(d) Will this representation be lossy, or perfectly preserve the data?

4. Sets of Eigenvectors

(a) Prove that if A is a symmetric matrix with n distinct eigenvalues, then its eigenvectors are orthogonal. Hint: if u and v are eigenvectors, calculate u^T Av two different ways.

(b) Suppose that A is a symmetric matrix. Prove, without appealing to calculus, that the solution to $\arg\max_x x^TAx$ s.t. $\|x\|_2 = 1$ is the eigenvector x_1 corresponding to the largest eigenvalue λ_1 of A. (Hint: the eigenvectors of a symmetric matrix can be chosen to be an orthonormal basis, i.e. unit vectors spanning all of $\mathbb{R}^n$.)

(c) Let A and B be two $\mathbb{R}^{n\times n}$ symmetric matrices. Suppose A and B have the exact same set of eigenvectors $\boldsymbol{u}_1, \boldsymbol{u}_2, \cdots, \boldsymbol{u}_n$ with the corresponding eigenvalues $\alpha_1, \alpha_2, \cdots, \alpha_n$ for $\boldsymbol{A}$, and $\beta_1, \beta_2, \cdots, \beta_n$ for $\boldsymbol{B}$. Please write down the eigenvectors and their corresponding eigenvalues for the following matrices:

(i) $D = A - B$

(ii) $E = AB$

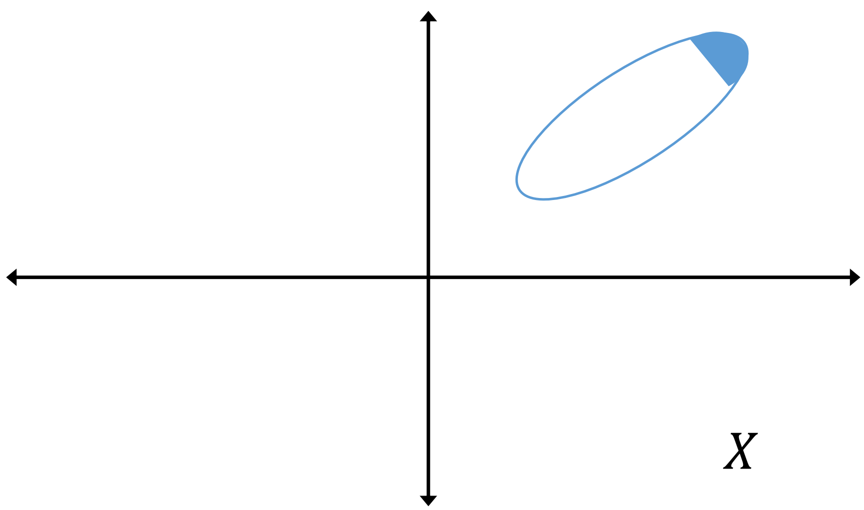
(iii) $\boldsymbol{F} = \boldsymbol{A}^{-1}\boldsymbol{B}$ (assume $\boldsymbol{A}$ is invertible)

5. Singular Value Decomposition - Whitening

We've seen before that demeaning our data makes it easier to work with. There's a more general operation called "whitening" where we also normalize the important directions of our data. In this problem, we'll do the operations corresponding to one version of whitening as a way to get better intuition on how SVD works.

Let $X \in \mathbb{R}^{n\times d}$ be a matrix of data points, and J be $\mathbf{I} - \mathbf{1}\mathbf{1}^T/n$. Let JX have a singular value decomposition of $JX = USV^T$.

Suppose we know that our points were drawn from a Gaussian distribution with covariance Σ. We would expect most of our points to lie in an ellipse, whose axes are the eigenvectors of Σ, scaled by the corresponding eigenvectors. We've drawn that ellipse below, with one area shaded so we can see its orientation.



For each of the following matrices:

- Verify that the resulting matrix is still $n \times d$, and therefore can be interpreted as modifying the datapoints of X
- Draw what the resulting data set would look like (i.e. how would the ellipse representing the covariance move?).

(a) JX

(b) JXV

(c) $JXVS^{-1}$, where S^{-1} is the $d \times d$ diagonal matrix, where $S^{-1}_{i,i} = 1/S_{i,i}$ (note that since S is not square, calling a matrix S^{-1} is an abuse of notation)

(d) $JXVS^{-1}V^T$