# 7 Principal Component Analysis

This topic will build a series of techniques to deal with high-dimensional data. Unlike regression problems, our goal is not to predict a value (the $y$-coordinate), it is to understand the "shape" of the data, for instance a low-dimensional representation that captures most of meaning of the high-dimensional data. This is sometimes referred to as *unsupervised learning* (as opposed to regression and classification, where the data has labels, known as supervised learning). Like most unsupervised settings, it can be a lot of fun, but its easy to get yourself into trouble if you are not careful.

We will cover many interconnected tools, including the singular value decomposition (SVD), eigenvectors and eigenvalues, the power method, principal component analysis, and multidimensional scaling.

## 7.1 Data Matrices

We will start with data in a matrix $A \in \mathbb{R}^{n \times d}$, and will call upon linear algebra to rescue us. It is useful to think of each row $a_i$ of $A$ as a data point in $\mathbb{R}^d$, so there are $n$ data points. Each dimension $j \in 1, 2, \ldots, d$ corresponds with an attribute of the data points.

**Example: Data Matrices**
There are many situations where data matrices arise.

- Consider a set of $n$ weather stations reporting temperature over $d$ points in time. Then each row $a_i$ corresponds to a single weather station, and each coordinate $A_{i,j}$ of that row is the temperature at station $i$ at time $j$.
- In movie ratings, we may consider $n$ users who have rated each of $d$ movies on a score of $1-5$. Then each row $a_i$ represents a user, and the $j$th entry of that user is the score given to the $j$ movie.
- Consider the price of a stock measured over time (say the closing price each day). Many time-series models consider some number of days ($d$ days, for instance 25 days) to capture the pattern of the stock at any given time. So for a given closing day, we consider the $d$ previous days. If we have data on the stock for 4 years (about 1000 days the stock market is open), then we can create a $d$-dimensional data points (the previous $d = 25$ days) for each day (except the first 25 or so). The data matrix is then comprised of $n$ data points $a_i$, where each corresponds to the closing day, and the previous $d$ days. The $j$th entry is the value on $(j-1)$ days before the closing day $i$.
- Finally consider a series of pictures of a shape (say the Utah teapot). The camera position is fixed as is the background, but we vary two things: the rotation of the teapot, and the amount of light. Here each pictures is a set of say $d$ pixels (say 10,000 if it is $100 \times 100$), and there are $n$ pictures. Each picture is a row of length $d$, and each pixel corresponds to a column of the matrix. Similar, but more complicated scenarios frequently occur with pictures of a persons face, or $3d$-imaging of an organ.

In each of these scenarios, there are many ($n$) data points, each with $d$ attributes. The following will be very important:

- **all coordinates have the same units!**

If this "same units" property does not hold, then when we measure a distance between data points in $\mathbb{R}^d$, usually using the $L_2$-norm, then the distance is nonsensical.

The next goal is to uncover a pattern, or a model $M$. In this case, the model will be a low-dimensional subspace $F$. It will represent a $k$-dimensional space, where $k << d$. For instance in the example with images, there are only two parameters which are changing (rotation, and lighting), so despite having $d = 10{,}000$ dimensions of data, 2 should be enough to represent everything.

### 7.1.1 Projections

Different than in linear regression this family of techniques will measure error as a projection from $a_i \in \mathbb{R}^d$ to the closest point $\pi_F(a_i)$ on $F$. To define this we will use linear algebra.

First recall, that given a unit vector $u \in \mathbb{R}^d$ and any data point $p \in \mathbb{R}^d$, then the dot product

$$\langle u, p \rangle$$

is the norm of $p$ projected onto the line through $u$. If we multiply this scalar by $u$ then

$$\pi_u(p) = \langle u, p \rangle u,$$

and it results in the point on the line through $u$ that is closest to data point $p$. This is a *projection of $p$ onto $u$*.

To understand this for a subspace $F$, we will need to define a basis. *For now we will assume that $F$ contains the origin $(0, 0, 0, \ldots, 0)$ (as did the line through $u$).* Then if $F$ is $k$-dimensional, then this means there is a $k$-dimensional basis $U_F = \{u_1, u_2, \ldots, u_k\}$ so that

- For each $u_i \in U_F$ we have $\|u_i\| = 1$, that is $u_i$ is a unit vector.
- For each pair $u_i, u_j \in U_F$ we have $\langle u_i, u_j \rangle = 0$; the pairs are orthogonal.
- For any point $x \in F$ we can write $x = \sum_{i=1}^{k} \alpha_i u_i$; in particular $\alpha_i = \langle x, u_i \rangle$.

Given such a basis, then the projection on to $F$ of a point $p \in \mathbb{R}^d$ is simply

$$\pi_F(p) = \sum_{i=1}^{k} \langle u_i, p \rangle u_i.$$

Thus if $p$ happens to be exactly in $F$, then this recovers $p$ exactly.

The other powerful part of the basis $U_F$ is the it defines a *new coordinate system*. Instead of using the $d$ original coordinates, we can use new coordinates $(\alpha_1(p), \alpha_2(p), \ldots, \alpha_k(p))$ where $\alpha_i(p) = \langle u_i, p \rangle$. To be clear $\pi_F(p)$ is still in $\mathbb{R}^d$, but there is a $k$-dimensional representation if we restrict to $F$.

When $F$ is $d$-dimensional, this operation can still be interesting. The basis we choose $U_F = \{u_1, u_2, \ldots, u_d\}$ could be the same as the original coordinate axis, that is we could have $u_i = e_i = (0, 0, \ldots, 0, 1, 0, \ldots, 0)$ where only the $i$th coordinate is 1. But if it is another basis, then this acts as a rotation (with possibility of also a mirror flip). The first coordinate is rotated to be along $u_1$; the second along $u_2$; and so on. In $\pi_F(p)$, the point $p$ does not change, just its representation.

### 7.1.2 SSE Goal

As usual our goal will be to minimize the sum of squared errors. In this case we define this as

$$\mathsf{SSE}(A, F) = \sum_{a_i \in A} \|a_i - \pi_F(a_i)\|^2,$$

and our desired $k$-dimensional subspace $F$ is

$$F^* = \arg\min_F \mathsf{SSE}(A, F)$$

As compared to linear regression, this is much less a "proxy goal" where the true goal was prediction. Now we have no labels (the $y_i$ values), so we simply try to fit a model through all of the data.

How do we solve for this?

- Linear regression does not work, its cost function is different.
- It is not obvious how to use gradient descent. The restriction that each $u_i \in U_F$ is a unit vector puts in a constraint, in fact a non-convex one. There are ways to deal with this, but we have not discussed these yet.
- ... linear algebra will come back to the rescue, now in the form of the SVD.

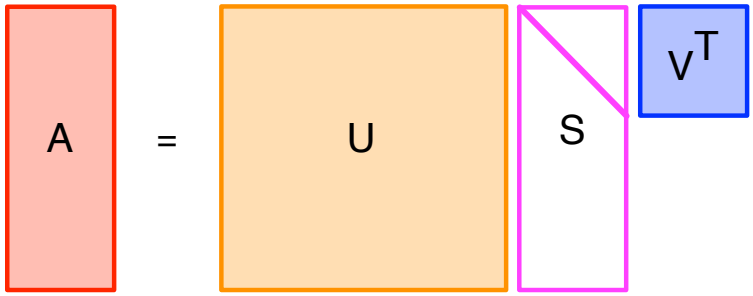
## 7.2 Singular Value Decomposition

A really powerful and useful linear algebra operation is called the *singular value decomposition*. It extracts an enormous amount of information about a matrix $A$. This section will define it and discuss many of its uses. Then we will describe one algorithm how to construct it. But in general, one simply calls the procedure in your favorite programming language and it calls the same highly-optimized back-end from the Fortran LAPACK library.

```
from scipy import linalg as LA
U, s, Vt = LA.svd(A)
```

The SVD takes in a matrix $A \in \mathbb{R}^{n \times d}$ and outputs three matrices $U \in \mathbb{R}^{n \times n}$, $S \in \mathbb{R}^{n \times d}$ and $V \in \mathbb{R}^{d \times d}$, so that $A = USV^T$.

$$[U, S, V] = \mathsf{svd}(A)$$



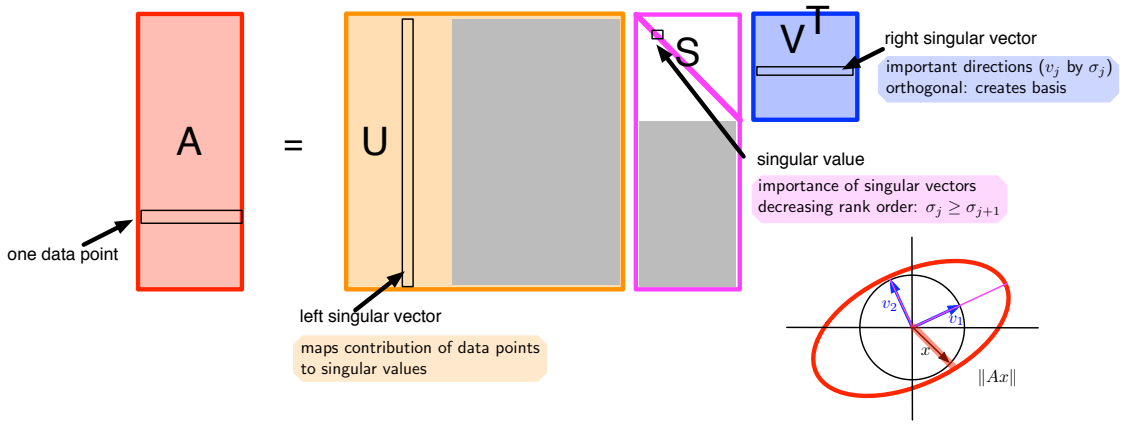

**The structure that lurks beneath.** The matrix $S$ only has non-zero elements along its diagonal. So $S_{i,j} = 0$ if $i \neq j$. The remaining values $\sigma_1 = S_{1,1}$, $\sigma_2 = S_{2,2}$, ..., $\sigma_r = S_{r,r}$ are known as the *singular values*. They have the property that

$$\sigma_1 \geq \sigma_2 \geq \ldots \sigma_r \geq 0$$

where $r \leq \min\{n, d\}$ is the rank of the matrix $A$. So the number of non-zero singular values reports the rank (this is a numerical way of computing the rank or a matrix).

The matrices $U$ and $V$ are orthogonal. Thus, their columns are all unit vectors and orthogonal to each other (within each matrix). The columns of $U$, written $u_1, u_2, \ldots, u_d$, are called the *left singular vectors*; and the columns of $V$, written $v_1, v_2, \ldots, v_n$, are called the *right singular vectors*.

This means for any vector $x \in \mathbb{R}^d$, the columns of $V$ (the right singular vectors) provide a basis. That is, we can write $x = \sum_{i=1}^{d} \alpha_i v_i$ for $\alpha_i = \langle x, v_i \rangle$. Similarly for any vector $y \in \mathbb{R}^n$, the columns of $U$ (the left singular vectors) provide a basis. This also implies that $\|x\| = \|V^T x\|$ and $\|y\| = \|yU\|$.




**Tracing the path of a vector.** To illustrate what this decomposition demonstrates, a useful exercise is to trace what happens to a vector $x \in \mathbb{R}^d$ as it is left-multiplied by $A$, that is $Ax = USV^T x$.

First $V^T x$ produces a new vector $\xi \in \mathbb{R}^d$. It essentially changes no information, just changes the basis to that described by the right singular values. For instance the new $i$ coordinate $\xi_i = \langle v_i, x \rangle$.

Next $\eta \in \mathbb{R}^n$ is the result of $SV^T x = S\xi$. It scales $\xi$ by the singular values of $S$. Note that if $d < n$ (the case we will focus on), then the last $n - d$ coordinates of $\eta$ are 0. In fact, for $j > r$ (where $r = \mathsf{rank}(A)$) then $\eta_j = 0$. For $j \leq r$, then the vector $\eta$ is stretched longer in the first coordinates since these have larger values.

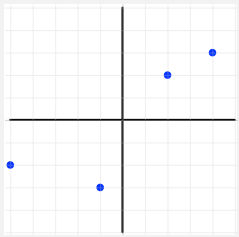
The final result is a vector $y \in \mathbb{R}^n$, the result of $Ax = USV^T x = U\eta$. This again just changes the basis of $\eta$ so that it aligns with the left singular vectors. In the setting $n > d$, the last $n - d$ left singular vectors are meaningless since the corresponding entries in $\eta$ are 0.

Working backwards ... this final $U$ matrix can be thought of mapping the effect of $\eta$ onto each of the data points of $A$. The $\eta$ vector, in turn, can be thought of as scaling by the content of the data matrix $A$ (the $U$ and $V^T$ matrices contain no scaling information). And the $\xi$ vector arises via the special rotation matrix $V^T$ that puts the starting point $x$ into the right basis to do the scaling (from the original $d$-dimensional coordinates to one that suits the data better).

**Example: Tracing through the SVD**

Consider a matrix

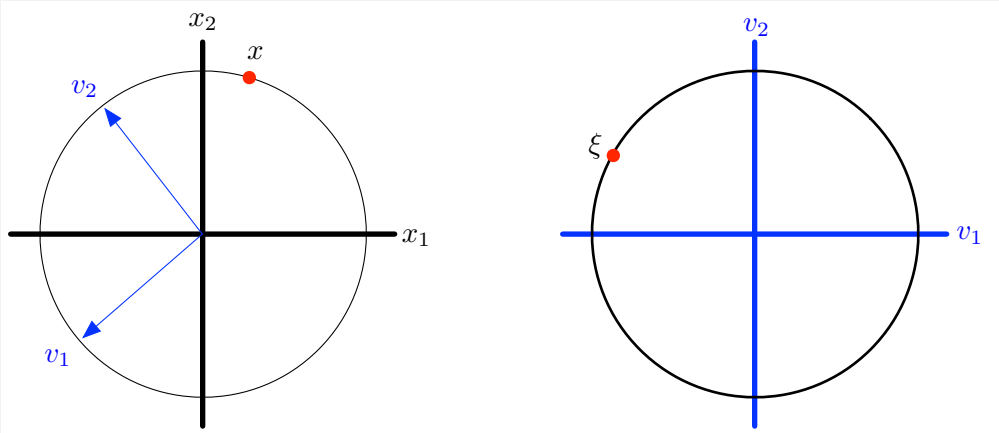
$$A = \begin{pmatrix} 4 & 3 \\ 2 & 2 \\ -1 & -3 \\ -5 & -2 \end{pmatrix},$$



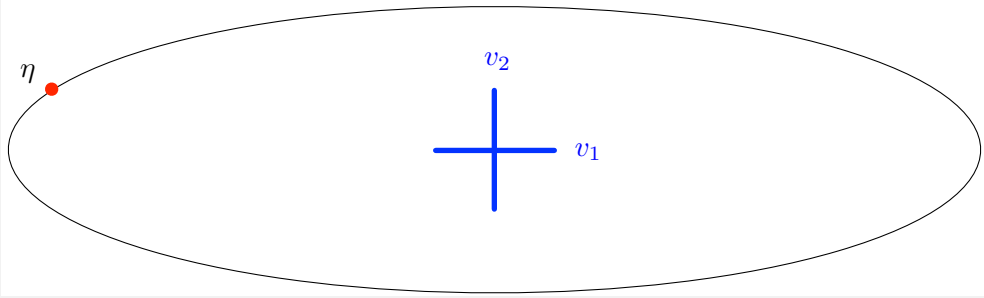
and its SVD $[U, S, V] = \mathsf{svd}(A)$:

$$U = \begin{pmatrix} -0.6122 & 0.0523 & 0.0642 & 0.7864 \\ -0.3415 & 0.2026 & 0.8489 & -0.3487 \\ 0.3130 & -0.8070 & 0.4264 & 0.2625 \\ 0.6408 & 0.5522 & 0.3057 & 0.4371 \end{pmatrix}, \quad S = \begin{pmatrix} 8.1655 & 0 \\ 0 & 2.3074 \\ 0 & 0 \\ 0 & 0 \end{pmatrix}, \quad V = \begin{pmatrix} -0.8142 & -.5805 \\ -0.5805 & 0.8142 \end{pmatrix}.$$

Now consider a vector $x = (0.243, 0.97)$ (scaled very slightly so it is a unit vector, $\|x\| = 1$). Multiplying by $V^T$ rotates (and flips) $x$ to $\xi = V^T x$; still $\|\xi\| = 1$




Next multiplying by $S$ scales $\xi$ to $\eta = S\xi$. Notice there are an imaginary third and fourth coordinates now; they are both coming out of the page! Don't worry, they won't poke you since their magnitude is 0.




Finally, $y = U\eta = Ax$ is again another rotation of $\eta$ in this four dimensional space.

```
import scipy as sp
import numpy as np
from scipy import linalg as LA


A = np.array([[4.0,3.0], [2.0,2.0], [-1.0,-3.0], [-5.0,-2.0]])

U, s, Vt = LA.svd(A, full_matrices=False)

print U
#[[-0.61215255 -0.05228813]
# [-0.34162337 -0.2025832 ]
# [ 0.31300005  0.80704816]
# [ 0.64077586 -0.55217683]]
print s
#[ 8.16552039  2.30743942]
print Vt
#[[-0.81424526 -0.58052102]
# [ 0.58052102 -0.81424526]]

x = np.array([0.243,0.97])
x = x/LA.norm(x)

xi = Vt.dot(x)
print xi
#[-0.7609864  -0.64876784]

S = LA.diagsvd(s,2,2)
eta = S.dot(xi)
print eta
#[-6.21384993 -1.49699248]

y = U.dot(eta)
print y
#[ 3.88209899  2.42606187 -3.1530804  -3.15508046]

print A.dot(x)
#[ 3.88209899  2.42606187 -3.1530804  -3.15508046]
```

### 7.2.1 Best Rank-$k$ Approximation

So how does this help solve the initial problem of finding $F^*$, which minimized the SSE? The singular values hold the key.

It turns out that there is a *unique* singular value decomposition, up to ties in the singular values. This means, there is exactly one (up to singular value ties) set of right singular values which rotate into a basis so that $\|Ax\| = \|SV^T x\|$ for all $x \in \mathbb{R}^d$ (recall that $U$ is orthogonal, so it does not change the norm, $\|U\eta\| = \|\eta\|$).

Next we realize that the singular values come in sorted order $\sigma_1 \geq \sigma_2 \geq \ldots \geq \sigma_r$. In fact, they are defined so that we choose $v_1$ so it maximizes $\|Av_1\|$, then we find the next singular vector $v_2$ which is orthogonal to $v_1$ and maximizes $\|Av_2\|$, and so on. Then $\sigma_i = \|Av_i\|$.

If we define $F$ with the basis $U_F = \{v_1, v_2, \ldots, v_k\}$, then

$$\|x - \pi_F(x)\|^2 = \left\| \sum_{i=1}^{d} v_i \langle x, v_i \rangle - \sum_{i=1}^{k} v_i \langle x, v_i \rangle \right\|^2 = \sum_{i=k+1}^{d} \langle x, v_i \rangle^2.$$

so the projection error is that part of $x$ in the last $(d-k)$ right singular vectors.

But we are not trying to directly predict new data here (like in regression). Rather, we are trying to approximate the data we have. We want to minimize $\sum_i \|a_i - \pi_F(a_i)\|^2$. But for any unit vector $u$, we recall now that

$$\|Au\|^2 = \sum_{i=1}^{n} \langle a_i, u \rangle.$$

Thus the projection error can be measured with a set of orthonormal vectors $w_1, w_2, \ldots, w_{d-k}$ which are each orthogonal to $F$, as $\sum_{j=1}^{n-k} \|Aw_j\|^2$. When defining $F$ as the first $k$ right singular values, then these orthogonal vectors are the remaining $(n-k)$ right singular vectors, so the projection error is

$$\sum_{i=1}^{n} \|a_i - \pi_F(a_i)\|^2 = \sum_{j=k+1}^{d} \|Av_j\|^2 = \sum_{j=k+1}^{d} \sigma_j^2.$$

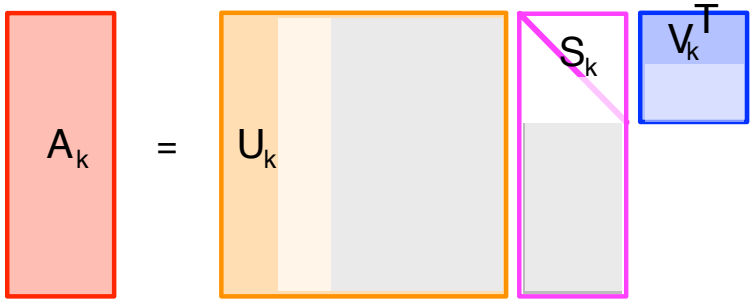
And thus by how the right singular vectors are defined, this expression is minimized when $F$ is defined as the span of the first $k$ singular values.

**Best rank-$k$ approximation.** A similar goal is to find the *best rank-$k$ approximation of $A$*. That is a matrix $A_k \in \mathbb{R}^{n \times d}$ so that $\mathsf{rank}(A_k) = k$ and it minimizes both

$$\|A - A_k\|_2 \quad \text{and} \quad \|A - A_k\|_F.$$

Note that $\|A - A_k\|_2 = \sigma_{k+1}$ and $\|A - A_k\|_F^2 = \sum_{j=k+1}^{d} \sigma_j^2$.

Remarkably, this $A_k$ matrix also comes from the SVD. If we set $S_k$ as the matrix $S$ in the decomposition so that all but the first $k$ singular values are 0, then it has rank $k$. Hence $A_k = US_kV^T$ also has rank $k$ and is our solution. But we can notice that when we set most of $S_k$ to 0, then the last $(d-k)$ columns of $V$ are meaningless since they are only multiplied by 0s in $US_kV^T$, so we can also set those to all 0s, or remove them entirely (along with the last $(d-k)$ columns of $S_k$). Similar we can make 0 or remove the last $(n-k)$ columns of $U$. These matrices are referred to as $V_k$ and $U_k$ respectively, and also $A_k = U_kS_kV_k^T$.



## 7.3 Eigenvalues and Eigenvectors

A related matrix decomposition to SVD is the eigendecomposition. This is only defined for a square matrix $B \in \mathbb{R}^{n \times n}$.

An *eigenvector* of $B$ is a vector $v$ such that there is some scalar $\lambda$ that

$$Bv = \lambda v.$$

That is, multiplying $B$ by $v$ results in a scaled version of $v$. The associated value $\lambda$ is called the *eigenvalue*. As a convention, we typically normalize $v$ so $\|v\| = 1$.

In general, a square matrix $B \in \mathbb{R}^{n \times n}$ may have up to $n$ eigenvectors (a matrix $\mathtt{V} \in \mathbb{R}^{n \times n}$) and values (a vector $\mathtt{l} \in \mathbb{R}^n$). Some of the eigenvalues may be complex numbers (even when all of its entries are real!).

```
from scipy import linalg as LA
l, V = LA.eig(B)
```

For this reason, we will focus on positive semidefinite matrices. A *positive definite matrix* $B \in \mathbb{R}^{n \times n}$ is a symmetric matrix with all positive eigenvalues. Another characterization is for every vector $x \in \mathbb{R}^n$ then $x^T B x$ is positive. A *positive semidefinite matrix* $B \in \mathbb{R}^{n \times n}$ may have some eigenvalues at 0 and are otherwise positive; equivalently for any vector $x \in \mathbb{R}^n$, then $x^T B x$ may be zero or positive.

How do we get positive semi-definite matrices? Lets start with a data matrix $A \in \mathbb{R}^{n \times d}$. Then we can construct two positive semidefinite matrices

$$B_R = A^T A \qquad \text{and} \qquad B_L = A A^T.$$

Matrix $B_R$ is $d \times d$ and $B_L$ is $n \times n$. If the rank of $A$ is $d$, then $B_R$ is positive definite. If the rank of $A$ is $n$, then $B_L$ is positive definite.

**Eigenvectors and eigenvalues relation to SVD.** Next consider the SVD of $A$ so that $[U, S, V] = \mathsf{svd}(A)$. Then we can write

$$B_R V = A^T A V = (VSU^T)(USV^T)V = VS^2.$$

Note that the last step follows because for orthogonal matrices $U$ and $V$, then $U^T U = I$ and $V^T V = I$, where $I$ is the identity matrix, which has no effect. The matrix $S$ is a diagonal square[1] matrix $S = \mathsf{diag}(\sigma_1, \sigma_2, \ldots, \sigma_d)$. Then $S^2 = SS$ (the product of $S$ with $S$) is again diagonal with entries $S^2 = \mathsf{diag}(\sigma_1^2, \sigma_2^2, \ldots, \sigma_d^2)$.

Now consider a single column $v_i$ of $V$ (which is the $i$th right singular vector of $A$). Then extracting this column's role in the linear system $B_R V = VS^2$ we obtain

$$B_R v_i = v_i \sigma_i^2.$$

This means that $i$th right singular vector of $A$ is an eigenvector (in fact the $i$th eigenvector) of $B_R = A^T A$. Moreover, the $i$th eigenvalue $\lambda_i$ of $B_R$ is the $i$th singular value of $A$ squared: $\lambda_i = \sigma_i^2$.

Similarly we can derive

$$B_L U = A A^T U = (USV^T)(VSU^T)U = US^2,$$

and hence the left singular vectors of $A$ are the eigenvectors of $B_L = AA^T$ and the eigenvalues of $B_L$ are the squared singular values of $A$.

[1] Technically, $S \in \mathbb{R}^{n \times d}$. To make this simple argument work, lets first assume w.l.o.g. (without loss of generality) that $d \leq n$. Then the bottom $n - d$ rows of $S$ are all zeros, which mean the right $n - d$ rows of $U$ do not matter. So we can ignore both these $n - d$ rows and columns. Then $S$ is square. This makes $U$ no longer orthogonal, so $U^T U$ is then a projection, not identity; but it turns out this is a project to the span of $A$, so the argument still works.

**Eigendecomposition.** In general, the eigenvectors provide a basis for a matrix $B \in \mathbb{R}^{n \times n}$ in the same way that the right $V$ or left singular vectors $U$ provide a basis for matrix $A \in \mathbb{R}^{n \times d}$. In fact, it is again a very special basis, and is unique up to the multiplicity of eigenvalues. This implies that all eigenvectors are orthogonal to each other.

Let $V = [v_1, v_2, \ldots, v_n]$ be the eigenvectors of the matrix $B \in \mathbb{R}^{n \times n}$, as columns in the matrix $V$. Also let $L = \mathsf{diag}(\lambda_1, \lambda_2, \ldots, \lambda_d)$ be the eigenvalues of $B$ stored on the diagonal of matrix $L$. Then we can decompose $B$ as

$$B = VLV^{-1}.$$

Note that the inverse of $L$ is $L^{-1} = \mathsf{diag}(1/\lambda_1, 1/\lambda_2, \ldots, 1/\lambda_n)$. Hence we can write

$$B^{-1} = VL^{-1}V^{-1}.$$

When $B$ is positive definite, it has $n$ positive eigenvectors and eigenvalues; hence $V$ is orthogonal, so $V^{-1} = V^T$. Thus in this situation, given the eigendecomposition, we now have a way to compute the inverse

$$B^{-1} = VL^{-1}V^T,$$

which was required in our almost closed-form solution for linear regression. Now we just need to compute the eigendecomposition, which we will discuss next.

## 7.4 The Power Method

The *power method* refers to what is probably the simplest algorithm to compute the first eigenvector and value of a matrix. By factoring out the effect of the first eigenvector, we can then recursively repeat the process on the remainder until we have found all eigenvectors and values. Moreover, this implies we can also reconstruct the singular value decomposition as well.

We will consider $B \in \mathbb{R}^{n \times n}$, a positive semidefinite matrix: $B = A^T A$.

**Algorithm 7.4.1** PowerMethod$(B, q)$

initialize $u^{(0)}$ as a random unit vector.
**for** $i = 1$ **to** $q$ **do**
  $u^{(i)} := Bu^{(i-1)}$
**return** $v := u^{(q)}/\|u^{(q)}\|$

We can unroll the for loop to reveal another interpretation. We can directly set $v^{(q)} = B^q v^{(0)}$, so all iterations are incorporated into one matrix-vector multiplication. Recall that $B^q = B \cdot B \cdot B \cdot \ldots \cdot B$, for $q$ times. However, these $q$ matrix multiplications are much more expensive then $q$ matrix-vector multiplications.

Alternatively we are provided only the matrix $A$ (where $B = A^T A$) then we can run the algorithm without explicitly constructing $B$ (since for instance if $d > n$ and $A \in \mathbb{R}^{n \times d}$, then the size of $B$ ($d^2$) may be much larger than $A$ ($nd$)). Then we simply replace the inside of the for-loop with

$$u^{(i)} := A^T(Au^{(i-1)})$$

where we first multiply $\tilde{u} = Au^{(i-1)}$ and then complete $u^{(i)} = A^T\tilde{u}$.

**Recovering all eigenvalues.** The output of PowerMethod$(B = A^T A, q)$ is a single unit vector $v$, which we will argue is arbitrarily close to the first eigenvector $v_1$. Clearly we can recover the first eigenvalue as

$\lambda_1 = \|Bv_1\|$. Since we know the eigenvectors form a basis for $B$, they are orthogonal. Hence, after we have constructed the first eigenvector $v_1$, we can factor it out from $B$ as follows:

$$A_1 := A - Av_1v_1^T B_1 := A_1^T A_1$$

Then we run PowerMethod($B_1 = A_1^T A_1, q$) to recover $v_2$, and $\lambda_2$; factor them out of $B_1$ to obtain $B_2$, and iterate.

**Why does the power method work?** To understand why the power method works, assume we know the eigenvectors $v_1, v_2, \ldots, v_n$ and eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_n$ of $B \in \mathbb{R}^{n \times n}$.

Since the eigenvectors form a basis for $B$, and assuming it is full rank, then also for all of $\mathbb{R}^n$ (if not, then it does not have $n$ eigenvalues, and we can fill out the rest of the basis of $\mathbb{R}^n$ arbitrarily). Hence, for any vector, including the initialization random vector $u^{(0)}$ can be written as

$$u^{(0)} = \sum_{j=1}^{n} \alpha_j v_j.$$

Recall that $\alpha_j = \langle u^{(0)}, v_j \rangle$, and since it is random, it is possible to claim that with probability at least $1/2$ that for any $\alpha_j$ we have that $|\alpha_j| \geq \frac{1}{2}\sqrt{n}$[2]. We will now assume that this holds for $j = 1$, so $\alpha_1 > 1/2\sqrt{n}$.

Next since we can interpret that algorithm as $v = B^q u^{(0)}$, then lets analyze $B^q$. If $B$ has $j$th eigenvector $v_j$ and eigenvalue $\lambda_j$, that is, $Bv_j = \lambda_j v_j$, then $B^q$ has $j$th eigenvalue $\lambda_j^q$ since

$$B^q v_j = B \cdot B \cdot \ldots \cdot Bv_j = B^{q-1}(v_j\lambda) = B^{q-2}(v_j\lambda)\lambda = v_j\lambda^q.$$

This holds for each eigenvalue of $B^q$. Hence we can rewrite output by summing over the terms in the eigenbasis as

$$v = \frac{\sum_{j=1}^{n} \alpha_j \lambda_j^q v_j}{\sqrt{\sum_{j=1}^{n} (\alpha_j \lambda_j^q)^2}}.$$

Finally, we would like to show our output $v$ is close to the first eigenvector $v_1$. We can measure closeness with the dot product (actually we will need to use its absolute value since we might find something close to $-v_1$).

$$\begin{aligned}
|\langle B^q u^{(0)}, v_1 \rangle| &= \frac{\alpha_1 \lambda_1^q}{\sqrt{\sum_{j=1}^{n} (\alpha_j \lambda_j^q)^2}} \\
&\geq \frac{\alpha_1 \lambda_1^q}{\sqrt{\alpha_1^2 \lambda_1^{2q} + n\lambda_2^{2t}}} \geq \frac{\alpha_1 \lambda_1^q}{\alpha_1 \lambda_1^q + \lambda_2^q \sqrt{n}} = 1 - \frac{\lambda_2^q \sqrt{n}}{\alpha_1 \lambda_1^q + \lambda_2^q \sqrt{n}} \\
&\geq 1 - 2\sqrt{n} \left(\frac{\lambda_2}{\lambda_1}\right)^q.
\end{aligned}$$

The first inequality holds because $\lambda_1 \geq \lambda_2 \geq \lambda_j$ for all $j > 2$. The third inequality (going to third line) holds by dropping the $\lambda_2^q \sqrt{n}$ term in the denominator, and since $\alpha_1 > 1/2\sqrt{n}$.

Thus if there is "gap" between the first two eigenvalues ($\lambda_1/\lambda_2$ is large), then this algorithm converges quickly to where $|\langle v, v_1 \rangle| = 1$.

[2]Since $u^{(0)}$ is a unit vector, its norm is 1, and because $\{v_1, \ldots, v_n\}$ is a basis, then $1 = \|u^{(0)}\|^2 = \sum_{j=1}^{n} \alpha_j^2$. Since it is random, then $\mathbf{E}[\alpha_j^2] = 1/n$ for each $j$. Applying a concentration of measure (almost a Markov Inequality, but need to be more careful), we can argue that with probability $1/2$ any $\alpha_j^2 > (1/4) \cdot (1/n)$, and hence $\alpha_j > (1/2) \cdot (1/\sqrt{n})$.

## 7.5 Principal Component Analysis

Recall that the original goal of this topic was to find the $k$-dimensional subspace $F$ to minimize

$$\|A - \pi_F(A)\|_F^2 = \sum_{a_i \in A} \|a_i - \pi_F(a_i)\|^2.$$

We have not actually solves this yet. The top $k$ right singular values $V_k$ of $A$ only provided this bound assuming that $F$ contains the origin: $(0, 0, \ldots, 0)$. However, this might not be the case!

*Principle Component Analysis (PCA)* is an extension of the SVD when we do not restrict that the subspace $V_k$ must go through the origin. It turns out, like with simple linear regression, that the optimal $F$ must go through the mean of all of the data. So we can still use the SVD, after a simple preprocessing step called centering to shift the data matrix so its mean is exactly at the origin.

Specifically, *centering* is adjusting the original input data matrix $A \in \mathbb{R}^{n \times d}$ so that each column (each dimension) has an average value of 0. This is easier than it seems. Define $\bar{a}_j = \frac{1}{n}\sum_{i=1}^n A_{i,j}$ (the average of each column $j$). Then set each $\tilde{A}_{i,j} = A_{i,j} - \bar{a}_j$ to represent the entry in the $i$th row and $j$th column of centered matrix $\tilde{A}$.

There is a *centering matrix* $C_n = I_n - \frac{1}{n}\mathbf{1}\mathbf{1}^T$ where $I_n$ is the $n \times n$ identity matrix, $\mathbf{1}$ is the all-ones column vector (of length $n$) and thus $\mathbf{1}\mathbf{1}^T$ is the all-ones $n \times n$ matrix. Then we can also just write $\tilde{A} = C_n A$.

Now to perform PCA on a data set $A$, we compute $[U, S, V] = \texttt{svd}(C_n A) = \texttt{svd}(\tilde{A})$.

Then the resulting singular values $\texttt{diag}(S) = \{\sigma_1, \sigma_2, \ldots, \sigma_r\}$ are known as the *principle values*, and the top $k$ right singular vectors $V_k = [v_1\ v_2\ \ldots\ v_k]$ are known as the top-$k$ *principle directions*.

This often gives a better fitting to the data than just SVD. The SVD finds the best rank-$k$ approximation of $A$, which is the best $k$-dimensional subspace (up to Frobenius and spectral norms) **which passes through the origin**. If all of the data is far from the origin, this can essentially "waste" a dimension to pass through the origin. However, we also need to store the shift from the origin, a vector $\tilde{c} = (\tilde{a}_1, \tilde{a}_2, \ldots, \tilde{a}_d) \in \mathbb{R}^d$.

## 7.6 Multidimensional Scaling

Dimensionality reduction is an abstract problem with input of a high-dimensional data set $P \subset \mathbb{R}^d$ and a goal of finding a corresponding lower dimensional data set $Q \subset \mathbb{R}^k$, where $k << d$, and properties of $P$ are preserved in $Q$. Both low-rank approximations through direct SVD and through PCA are examples of this: $Q = \pi_{V_k}(P)$. However, these techniques require an explicit representation of $P$ to start with. In some cases, we are only presented $P$ more abstractly. There two common situations:

- We are provided a set of $n$ objects $X$, and a bivariate function $\texttt{d} : X \times X \to \mathbb{R}$ that returns a distance between them. For instance, we can put two cities into an airline website, and it may return a dollar amount for the cheapest flight between those two cities. This dollar amount is our "distance."
- We are simply provided a matrix $D \in \mathbb{R}^{n \times n}$, where each entry $D_{i,j}$ is the distance between the $i$th and $j$th point. In the first scenario, we can calculate such a matrix $D$.

*Multi-Dimensional Scaling* (MDS) has the goal of taking such a distance matrix $D$ for $n$ points and giving low-dimensional (typically) Euclidean coordinates to these points so that the embedded points have similar spatial relations to that described in $D$. If we had some original data set $A$ which resulted in $D$, we could just apply PCA to find the embedding. It is important to note, in the setting of MDS we are typically just given $D$, and *not* the original data $A$. However, as we will show next, we can derive a matrix that will act like $AA^T$ using only $D$.

A *similarity matrix* $M$ is an $n \times n$ matrix where entry $M_{i,j}$ is the similarity between the $i$th and the $j$th data point. The similarity often associated with Euclidean distance $\|a_i - a_j\|$ is the standard inner (or dot

product) $\langle a_i, a_j \rangle$. We can write

$$\|a_i - a_j\|^2 = \|a_i\|^2 + \|a_j\|^2 - 2\langle a_i, a_j \rangle,$$

and hence

$$\langle a_i, a_j \rangle = \frac{1}{2}\left(\|a_i\|^2 + \|a_j\|^2 - \|a_i - a_j\|^2\right). \tag{7.1}$$

Next we observe that for the $n \times n$ matrix $AA^T$ the entry $[AA^T]_{i,j} = \langle a_i, a_j \rangle$. So it seems hopeful we can derive $AA^T$ from $D$ using equation (7.1). That is we can set $\|a_i - a_j\|^2 = D_{i,j}^2$. However, we need also need values for $\|a_i\|^2$ and $\|a_j\|^2$.

Since the embedding has an arbitrary shift to it (if we add a shift vector $s$ to *all* embedding points, then no distances change), then we can arbitrarily choose $a_1$ to be at the origin. Then $\|a_1\|^2 = 0$ and $\|a_j\|^2 = \|a_1 - a_j\|^2 = D_{1,j}^2$. Using this assumption and equation (7.1), we can then derive the similarity matrix $AA^T$. Then we can run the eigen-decomposition on $AA^T$ and use the coordinates of each point along the first $k$ eigenvectors to get an embedding. This is known as *classical MDS*.

It is often used for $k$ as 2 or 3 so the data can be easily visualized.

There are several other forms that try to preserve the distance more directly, where as this approach is essentially just minimizing the squared residuals of the projection from some unknown original (high-dimensional embedding). One can see that we recover the distances with no error if we use all $n$ eigenvectors – if they exist. However, as mentioned, there may be less than $n$ eigenvectors, or they may be associated with complex eigenvalues. So if our goal is an embedding into $k = 3$ or $k = 10$, there is no guarantee that this will work, or even what guarantees this will have. But MDS is used a lot nonetheless.