Unit 3: Spectral Theorem: EVD and SVD

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Contents

In this chapter, we will cover the so-called spectral theorem, which is one of the main results in linear algebra, and which is central to a lot of applications of linear algebra, including in data science.

Here, we will discuss the spectral theorem in the form of the EVD of a symmetric matrix, and we will also discuss the extension of it known as the SVD.

1 Spectral theorem

To start, the spectral theorem is called the spectral theorem since it has to do with the eigenvalues and eigenvectors of a matrix. Recall that the set of eigenvalues of a matrix has a special name.

Definition. The set of eigenvalues of a matrix is called the **spectrum** of a matrix.

Eigenspaces

Earlier we have discussed the following four thorems:

> **Theorem 1.6.** An orthogonal set of nonzero vectors in a vector space is linearly independent.
>
> **Theorem 7.1** (Spectral decomposing I) Let v_1, v_2 be the eigenvectors associated with the eigenvalues λ_1, λ_2 of a 2×2 symmetric matrix A respectively. If
>
> $$\Lambda = \begin{pmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{pmatrix}, \qquad V = (v_1 \quad v_2),$$

then

$$A = V\Lambda V^T.$$

Theorem 8.1. If a matrix A is symmetric, then any two distinct eigenvectors corresponding to different eigenvalues are orthogonal.

Theorem 8.2. If A is a symmetric matrix, then all eigenvalues of A are real. (Without proof)

If v and w are eigenvectors associated with the same eigenvalue λ, then

$$A(v + w) = Av + Aw = \lambda v + \lambda w = \lambda(v + w)$$

and for any realnumber c,

$$A(cv) = c(Av) = c(\lambda v) = \lambda(cv).$$

Hence a set containing

- all eigenvectors associated with λ and
- the zero vector.

is a well-defined subspace of $\mathbb{R}^n$.We shall call it an **eigenspace** associated with the eigenvalue λ. The dimension of this space is called the **geometric multiplicity** of λ.

Theorem 1.1. *If an $n \times n$ matrix A is nonsingular, then the columns of A are linearly independent.*

Proof. With $v_1, ..., v_n$ referring to the columns of A, the equation

$$x_1v_1 + ... + x_nv_n = 0$$

can be rewritten as

$$Ax = 0.$$

Now, by assumption, A is nonsingular. So, it is invertible. We want to show that the only solution to $Ax = 0$ is $x = 0$. Multiplying both sides by A^{-1} gives us

$$Ax = 0 \Rightarrow A^{-1}Ax = A^{-1}0 \Rightarrow x = 0$$

So, we may indeed state that the only x with $Ax = 0$ is the vector $x = 0$. Therefore, $v_1, ..., v_n$ are linearly independent. ◀

Definition. A matrix A is said to be **diagonalizable**, if there is a nondingular matrix P and a diagonal matrix D such that

$$A = PDP^{-1}.$$

Theorem 1.2. *Let $\{v_1, v_2, ..., v_k\}$ be a linearly independent set of eigenvectors of an $n \times n$ matrix A, extend it to a basis $\{v_1, v_2, ..., v_k, ..., v_n\}$ of $\mathbb{R}^n$, and let*

$$P = (v_1 \ v_2 \ ... \ v_n)$$

be the (invertible) $n \times n$ matrix. If $\lambda_1, \lambda_2, ..., \lambda_k$ are the (not necessarily distinct) eigenvalues of A corresponding to $v_1, v_2, ..., v_k$ respectively, then $P^{-1}AP$ has block form:

$$P^{-1}AP = \begin{pmatrix} \operatorname{diag}(\lambda_1, ..., \lambda_k) & B \\ 0 & A_1 \end{pmatrix},$$

where B has size $k \times (n-k)$ and A_1 has size $(n-k) \times (n-k)$.

Proof. If $\{e_1, e_2, ..., e_n\}$ is the standard basis for $\mathbb{R}^n$, then

$$\begin{aligned}(e_1 \ ... \ e_n) = I_n = P^{-1}P &= P^{-1}(v_1 \ ... \ v_n) \\ &= (P^{-1}v_1 \ ... \ P^{-1}v_n).\end{aligned}$$

Comparing columns, we have $P^{-1}v_i = e_i$ for each $1 \leq i \leq n$. On the other hand, observe that

$$P^{-1}AP = P^{-1}A(v_1 \ ... \ v_n) = ((P^{-1}A)v_1 \ ... \ (P^{-1}A)v_n).$$

Hence, if $1 \leq i \leq k$, column i of $P^{-1}AP$ is

$$(P^{-1}A)v_i = P^{-1}(\lambda_i v_i) = \lambda_i P^{-1}(v_i) = \lambda_i e_i.$$

This describes the first k columns of $P^{-1}AP$, and the theorem follows. ◀

Theorem 1.3. *Let A be an $n \times n$ matrix.*

1. *A is diagonalizable if and only if it has eigenvectors $v_1, ..., v_n$ such that the matrix $P = (v_1 \ ..., \ v_n)$ is invertible*
2. *When this is the case, $P^{-1}AP = \operatorname{diag}(\lambda_1, ..., \lambda_n)$ where, for each i, λ_i is the eigenvalue of A corresponding to v_i.*

Theorem 1.4. *Let A be an $n \times n$ matrix. A is diagonalizable if and only if it has n linearly independent eigenvectors.*

Proof. " $\Rightarrow$ " Let A be diagonalizable. Then there is a non-singular matrix P and a diagonal matrix D such that

$$A = PDP^{-1}$$

so that

$$AP = PD.$$

We can specify columns of P and entries of D in this equation

$$A(v_1 \ ..., \ v_n) = (v_1 \ ..., \ v_n) \begin{pmatrix} d_1 & & 0 \\ & \ddots & \\ 0 & & d_n \end{pmatrix},$$

where the column vectors $v_1, ..., v_n$ are the columns of A. Then we have

$$(Av_1\ ...,\ Av_n) = (d_1v_1\ ...,\ d_nv_n).$$

This gives

$$Av_i = d_iv_i$$

for all $i \in \{1, ..., n\}$. That means, $v_1, ..., v_n$ eigenvectors associated with the eigenvalues $\lambda_1 = d_1, ..., \lambda_n = d_n$ respectively associated with A. Moreover, by assumption, P is nonsingular. Then $v_1, ..., v_n$, being the columns of P, are linearly independent. Therefore, A has n linearly independent eigenvectors.

" $\Rightarrow$ " Assume that A has n linearly independent eigenvectors $v_1, ..., v_n$ associated with the eigenvalues $\lambda_1, ..., \lambda_n$ respectively. Then

$$Av_i = \lambda_iv_i,$$

Rewriting these in the matrix form, we obtain

$$\begin{aligned} & AP = P\Lambda \\ \Rightarrow \quad & A = P\Lambda P^{-1}, \end{aligned}$$

where

$$\Lambda = \begin{pmatrix} \lambda_1 & & 0 \\ & \ddots & \\ 0 & & \lambda_n \end{pmatrix}.$$

Since the columns of the $n \times n$ matrix P are linearly independent, P is nonsingular. Hence A is diagonalizable. ◀

Theorem 1.5. *A square matrix A is diagonalizable if and only if every eigenvalue λ of multiplicity m yields exactly m basic eigenvectors.*

In particular,

Theorem 1.6. *An $n \times n$ matrix with n distinct eigenvalues is diagonalizable.*

Moreover, the matrix V with these eigenvectors as columns is a diagonalizing matrix for A, that is,

$$P^{-1}AP \text{ is diagonal.}$$

As we have seen, the really nice bases of $\mathbb{R}^n$ are the orthogonal ones, so a natural question is: which $n \times n$ matrices have an orthogonal basis of eigenvectors? These turn out to be precisely the symmetric matrices.

Definition. An $n \times n$ matrix A is said to be **orthogonally diagonalizable** when an orthogonal matrix P can be found such that $P^{-1}AP = P^T AP$ is diagonal.

If the matrix is symmetric, the eigendecomposition of the matrix could actually be a very simple yet useful form.

Theorem 1.7. *If an $n \times n$ matrix A is orthogonally diagonalizable, then A is a symmetric matrix.*

Proof. If A is orthogonally diagonalizable, then

$$A^T = (PDP^T)^T = P^{TT} D^T P^T = PDP^T = A.$$

Thus, A is symmetric. ◀

Its convers is also true.

Theorem 1.8. *If an $n \times n$ matrix A is symmetric, then A is orthogonally diagonalizable.*

Theorem 1.9 (Principal Axes Theorem)**.** *The following conditions are equivalent for an $n \times n$ matrix A.*

1. *A has an orthonormal set of n eigenvectors.*
2. *A is orthogonally diagonalizable.*
3. *A is symmetric.*

If we are willing to replace "diagonal" by "upper triangular" in the principal axes theorem, we have the following result.

Theorem 1.10. *Let A be a real $n \times n$ matrix. If A is symmetric, then there is an orthogonal matrix U and an upper triangular matrix T such that $A = UTU^T$.*

Proof. Let v_1 be an eigenvector of norm 1, with eigenvalue λ_1. Let $u_2, ..., u_n$ be any orthonormal vectors orthogonal to v_1. Put $U_1 = \{v_1, u_2, ..., u_n\}$. Then $U_1^T U_1 = I$, and

$$U_1^T A U_1 = \begin{pmatrix} \lambda_1 & \cdots \\ 0 & A_2 \end{pmatrix}.$$

Now we claim that A_2 has eigenvalues $\lambda_2, ..., \lambda_n$. This is true because

$$\begin{aligned} |A - \lambda I| &= |U_1^T||A - \lambda I||U_1| = |U_1^T(A - \lambda I)U_1| \\ &= |U_1^T A U_1 - \lambda U_1^T U_1| \\ &= \begin{vmatrix} \lambda_1 - \lambda & \cdots \\ 0 & A_2 - \lambda I \end{vmatrix} \\ &= (\lambda_1 - \lambda)|A_2 - \lambda I|. \end{aligned}$$

So A_2 has real eigenvalues, namely, $\lambda_2, ..., \lambda_n$. Now we proceed by induction.

Suppose we have proved the theorem for $n = k$. Then we use this fact to prove the theorem is true for $n = k + 1$. Note that the theorem is trivial if $n = 1$.

So for $n = k + 1$, we proceed as above and then apply the known theorem to A_2, which is $k \times k$. We find that $A_2 = U_2 T_2 U^T$. Now this is the hard part. Let U_1 and A_2 be as above, and let

$$U = U_1 \begin{pmatrix} 1 & 0 \\ 0 & U_2 \end{pmatrix}.$$

Then

$$\begin{aligned} AU &= AU_1 \begin{pmatrix} 1 & 0 \\ 0 & U_2 \end{pmatrix} = U_1 \begin{pmatrix} \lambda_1 & \cdots \\ 0 & A_2 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & U_2 \end{pmatrix} \\ &= U_1 \begin{pmatrix} \lambda_1 & \cdots \\ 0 & A_2 U_2 \end{pmatrix} = U_1 \begin{pmatrix} \lambda_1 & \cdots \\ 0 & U_2 T_2 \end{pmatrix} \\ &= U_1 \begin{pmatrix} 1 & 0 \\ 0 & U_2 \end{pmatrix} \begin{pmatrix} \lambda_1 & \cdots \\ 0 & T_2 \end{pmatrix} = UT, \end{aligned}$$

where T is upper triangular. So $AU = UT$, or $A = UTU^T$. ◀

Theorem 1.11. *Let A be a real $n \times n$ matrix. If $U^T AU = D$, where U is orthogonal and D is diagonal, then A is a symmetric matrix.*

Proof. Suppose that $U^T AU = D$, where U is orthogonal and D is diagonal. Since D is diagonal, we know that $D^T = D$. Thus, using the transpose operation on the equality $U^T AU = D$, we obtain

$$U^T AU = D = D^T = (U^T AU)^T = U^T A^T U.$$

From this result, we see that $U^T AU = U^T A^T U$. Multiplying by

U and U^T , we obtain

$$\begin{aligned} & U(U^TAU)U^T = U(U^TA^TU)U^T \\ \Rightarrow \quad & (UU^T)A(UU^T) = (UU^T)A^T(UU^T) \\ \Rightarrow \quad & A = A^T. \end{aligned}$$

Thus,the matrix A is symmetric. ◀

2 Spectral Theorem for Symmetric Matrices

Theorem 2.1 (Spectral Theorem for Symmetric Matrices)**.**

(a) *A has n real eigenvalues, including multiplicity.*

(b) *For each distinct eigenvalue, there is an associated eigenspace, and the dimension of the eigenspace is the multiplicity of the corresponding eigenvalue as the root of the characteristic equation.*

(c) *Eigenspaces corresponding to distinct eigenvalues are mutually orthogonal.*

(d) *A is orthogonally diagonalizable.*

As given above, the form of the spectral theorem restricted to symmetric real-valued matrices is sometimes called the **Eigen-Value Decomposition** (EVD).

3 EigenValue Decomposition

3.1 Efficiently Expressing the EVD

Assume that we have n eigenvalues. Then we obtain n eigen euqtions:

$$Au_i = \lambda_i u_i \quad \text{for } i \in \{1, 2, ..., n\}.$$

We can express them efficiently writing in the matrix form as follows:

$$AU = U\Lambda, \tag{1}$$

where Λ is the diagonal matrix of eigenvalues λ_i's arranged in decreasing order and U is the $n \times n$ orthogonal matrix of the eigenvectors associated with the eigenvalues λ_i's.

The spectral decomposition.

Note that since U is orthogonal, we have $U^{-1} = U^T$.

There are two complementary ways to view Equation (1):

1. We can rewrite Equation (1) as follows:

$$A = U\Lambda U^T. \tag{2}$$

   This equation provides a decomposition of A as a product of three matrices.

2. We can also rewrite Equation (1) as follows:

$$U^T AU = \Lambda. \tag{3}$$

   This equation expresses A in the rotated basis defined by U. The point is that in the complete orthonormal basis of eigenvectors, the matrix A is a diagonal matrix, with diagonal elements equal to the eigenvalues.

From Equation 2, we get

$$
\begin{aligned}
A &= (u_1 \ldots u_n) \begin{pmatrix} \lambda_1 & & 0 \\ & \ddots & \\ 0 & & \lambda_n \end{pmatrix} \begin{pmatrix} u_1^T \\ \vdots \\ u_n^T \end{pmatrix} \\
&= (\lambda_1 u_1 \ldots \lambda_n u_n) \begin{pmatrix} u_1^T \\ \vdots \\ u_n^T \end{pmatrix} \\
&= \sum_{i=1}^{n} \lambda_i u_i u_i^T .
\end{aligned}
$$

Thus, we have expressed the matrix A as a sum of rank-1 matrices, each of which was the outer product of an eigenvector with its transpose, and each of which is scaled by its associated eigenvalue.

Definition. This last equation, equivalently either (2) or (3), is the spectral decomposition of the matrix A. Each term, $\lambda_i u_i u_i^T$ is an $n \times n$ matrix of rank 1, and $\lambda_i u_i u_i^T x$ orthogonal projection of the vector x onto the span of u_i.

Example 1.

Determine the spectral decomposition of the matrix associated with the quadratic form:

$$5x_1^2 - 4x_1x_2 + 5x_2^2 = 48.$$

Solution. Let's rewrite the quadratic form as a matrix equation,

$$(x_1 \; x_2) \begin{pmatrix} 5 & -2 \\ -2 & 5 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = 48.$$

This is a symmetric matrix, and so we know it has a full set of eigenvectors and eigenvalues. Let's compute (recompute) them. To do so, compute

$$\begin{aligned} 0 = |A - \lambda I| &= \begin{vmatrix} 5-\lambda & -2 \\ -2 & 5-\lambda \end{vmatrix} \\ &= (5-\lambda)^2 - 4 \\ &= \lambda^2 - 10\lambda + 21 \\ &= (\lambda - 7)(\lambda - 3). \end{aligned}$$

So, the two distinct eigenvalues are $\lambda_1 = 7$ and$\lambda_2 = 3$.

<u>For $\lambda_1 = 7$</u>, we have

$$\begin{pmatrix} -2 & -2 \\ -2 & -2 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}.$$

Clearly, the eigenvector associated with λ_1 is

$$v_1 = \begin{pmatrix} 1/\sqrt{2} \\ -1/\sqrt{2} \end{pmatrix}.$$

<u>For $\lambda_2 = 3$</u>, we have

$$\begin{pmatrix} 2 & -2 \\ -2 & 2 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}.$$

Clearly, the eigenvector associated with λ_2 is

$$v_2 = \begin{pmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \end{pmatrix}.$$

Set

$$\begin{aligned} V &= (v_1\ v_2) = \begin{pmatrix} 1/\sqrt{2} & 1/\sqrt{2} \\ -1/\sqrt{2} & 1/\sqrt{2} \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix}, \\ \Lambda &= \begin{pmatrix} 7 & 0 \\ 0 & 3 \end{pmatrix}. \end{aligned}$$

Then

$$
\begin{aligned}
V\Lambda V^T &= \frac{1}{2}\begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix}\begin{pmatrix} 7 & 0 \\ 0 & 3 \end{pmatrix}\begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix} \\
&= \frac{1}{2}\begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix}\begin{pmatrix} 7 & -7 \\ 3 & 3 \end{pmatrix} \\
&= \frac{1}{2}\begin{pmatrix} 10 & -4 \\ -4 & 10 \end{pmatrix} \\
&= \begin{pmatrix} 5 & -2 \\ -2 & 5 \end{pmatrix}.
\end{aligned}
$$

Therefore,

$$A = V\Lambda V^T.$$

3.2 Finding the EVD

(a) Eigenvalues/eigenvectors as optimization problems. Let's consider the problem:

$$\text{Find } x \in \mathbb{R}^n \text{ to attain} \quad \max x^T A x,$$

i.e., find the vector that gives the largest value of the quadratic form associated with the matrix.

Unfortunately, this problem isn't well-defined in the sense that it doesn't (or, more precisely, depending on A, it (may not) have a maximum: given any vector x, we can increase the value of the objective by considering the vector $x' = 2x$.

The way to avoid this issue is to "constrain" $x \in \mathbb{R}^n$. By this, we mean that we want to consider not all $x \in \mathbb{R}^n$, but only a subset of all possible x, and in particular a subset that does not permit us to consider scaling x arbitrarily by $\alpha \in \mathbb{R}^+$. There are many ways to constrain x, but the one that leads to the spectral decomposition is to constrain x to the unit ball in $\mathbb{R}^n$. That is, we try to solve the problem

$$\text{Find } x \in \mathbb{R}^n \text{ to attain} \quad \max x^T A x \quad \text{s.t. } x^T x = 1.$$

That is, we consider all vectors on the unit ball in $\mathbb{R}^n$, i.e., we consider all directions but we don't worry about magnitudes, and we ask ourselves which direction has the largest value of this quadratic function. The solution of this objective is the first eigenvalue; moreover, the vector achieving it is the first eigenvector. (That discussion assumes uniqueness of eigenvalues, and as usual we have the usual issues come up if there is multiplicity, but let's assume that for now.)

The above problem can also be written as

$$\text{Find} \quad \arg\max_{x \in \mathbb{R}^n} x^T A x \quad \text{s.t. } x^T x = 1.$$

(b) Optimization and constrained optimization Let's consider the next most simple case. In this case, we have a function $f(x_1, x_2) = x^T A x$, i.e., where $x \in \mathbb{R}^2$. In this case, the constraint means that we choose the unit Euclidean ball $x^T x = x_1^2 + x_2^2 = 1$. To do this in a way that generalizes to $\mathbb{R}^3$ and beyond requires some machinery.

(c) Method of Lagrange Multipliers. The general way to deal with a constrained optimization problem is to consider the **method of Lagrange Multipliers**. This is an approach to convert a constrained optimization problem, e.g., an optimization problem with equality constraints, into an unconstrained optimization problem where the first and second order conditions can be applied. It does so by replacing the constrained optimization problem by introducing a new variable and converting it to an unconstrained optimization problem.

Example 2.

Consider the following problem:

$$\begin{aligned} &\text{Minimize} \quad f(x_1, x_2) \\ &\text{subject to} \quad g(x_1, x_2) = 0. \end{aligned}$$

Let's introduce a parameter $\lambda \in \mathbb{R}$ and define the following function:

$$L = L(x_1, x_2, \lambda) = f(x_1, x_2) - \lambda g(x_1, x_2).$$

The function L is called the **Lagrangian**.

Fact. If $f(x_1^*, x_2^*)$ is the maximum of $f(x_1, x_2)$ such that $g(x_1, x_2) = 0$, then there exists a $\lambda*$ such that (x_1, x_2, λ) is a stationary point of the Lagrangian function L.

At that stationary point, all the first derivatives of L equal zero.

Caveat. It is NOT the case that all stationary points of the Lagrangian solve the original problem. There are technical necessary and sufficient conditions for all this to go through. We won't go through all that here (you need a more advanced class for that), but those conditions will hold in the examples to which we will apply it.

In the 2-dimensional case,

$$f(x_1, x_2) = a_{11}x_1^2 + (a_{12} + a_{21})x_1x_2 + a_{22}x_2^2,$$

in which the derivatives with respect to x_1 and x_2 are

$$\frac{\partial f}{\partial x_1} = 2a_{11}x_1 + (a_{12} + a_{21})x_2$$
$$\frac{\partial f}{\partial x_2} = (a_{12} + a_{21})x_1 + 2a_{22}x_2,$$

which can be written in more compact notation as

$$\frac{\partial f}{\partial x} = \begin{pmatrix} \frac{\partial f}{\partial x_1} \\ \frac{\partial f}{\partial x_2} \end{pmatrix} = \begin{pmatrix} 2a_{11} & a_{12} + a_{21} \\ a_{12} + a_{21} & 2a_{22} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = 2Ax.$$

So, in the 2-dimensional case, we want to optimize

$$\begin{aligned} &\text{Minimize} \quad x^T Ax \\ &\text{subject to} \quad x^T x = 1. \end{aligned}$$

Thus, in this case, the Lagrangian is

$$L = L(x_1, x_2, \lambda) = L(x, \lambda) = x^T Ax - \lambda(x^T x - 1).$$

<u>Note here that</u> the term multiplying the λ is $(x^T x - 1)$ and not $x^T x$. The reason for this is that the constraint is $x^T x = 1$, and so to convert it to a form $g(x) = 0$, we need to have $g(x) = x^T x - 1$. Don't forget to do this. Now, consider the problem of finding

$$\min_{x,\lambda} x^T Ax - \lambda(x^T x - 1),$$

where this is now an unconstrained optimization problem, and thus we can apply the usual first and second order conditions to it.

We have derived this by considering $x \in \mathbb{R}^2$, but nothing in its derivation needs to be just 2-dimensional (and nothing in what follows needs that either). For example, the expression

$$\frac{\partial f}{\partial x} = 2Ax$$

generalizes to n dimensions.

In particular, the function we are interested in more generally is $f(x) = x^T A x$, where

$$x \in \mathbb{R}^n, \ A \in \mathbb{R}^{n \times n}, \ f(x) \in \mathbb{R}.$$

(d) Derivatives of functions in higher dimensions.

Many of the rules from one-dimensional calculus generalize to functions that involve many variables. There are some things that are different, but the following things are good to know.

Let A be an $n \times n$ matrix (square, but not necessarily symmetric), let $a \in \mathbb{R}^n$ be a column vector (i.e., an $n \times 1$ matix), and let $x \in \mathbb{R}^n$ be a column vector of variables. Then, we can show the following.

- If $z = a^T x$, then

$$\frac{\partial z}{\partial x} = \frac{\partial a^T x}{\partial x} = a.$$

- If $z = x^T x$, then

$$\frac{\partial z}{\partial x} = \frac{\partial x^T x}{\partial x} = 2x.$$

- If $z = a^T Ax$, then

$$\frac{\partial z}{\partial x} = \frac{\partial a^T Ax}{\partial x} = A^T a.$$

- If $z = x^T Ax$, then

$$\frac{\partial z}{\partial x} = \frac{\partial x^T Ax}{\partial x} = Ax + A^T x.$$

If, in addition, A is symmetric, then

$$\frac{\partial z}{\partial x} = \frac{\partial x^T Ax}{\partial x} = 2Ax.$$

In these expressions, $\frac{\partial}{\partial x}$ is a derivative operator that can be applied to a function and that yields slighlty different results depending on the form of the function to which it is applied. In particular, it can be applied to a function

$$f(x) = f(x_1, ..., x_n),$$

(i.e., a function that takes as input a vector x and) that returns as output a scalar or a vector.

- If $f(x) \in \mathbb{R}$, then

$$\frac{\partial f}{\partial x} = \left(\frac{\partial f}{\partial x_1}\ ,\ \dots\ ,\ \frac{\partial f}{\partial x_n} \right) \in \mathbb{R},$$

  i.e., it returns a vector, the ith element of which is the function differentiated with respect to the ith variable. That is, the derivative of a scalar-valued function of a vector input is itself a vector, the elements of which encode the derivative information of the output with respect to each element of the input. (For one-dimensional functions, derivatives are basically linear approximations of the function, as the input variable changes. So too, here, derivatives are linear approximations, but the linear approximation is in $\mathbb{R}^n$, since the input can vary in $\mathbb{R}^n$.) As with other vectors, this can be interpreted as a direction in $\mathbb{R}^n$ and a magnitude in that direction.

- If $f(x) = (f_1(x), ..., f_m(x)) \in \mathbb{R}^m$, then it returns an $m \times n$ matrix

$$\begin{pmatrix} \frac{\partial f_1}{\partial x_1} & \cdots & \frac{\partial f_1}{\partial x_n} \\ \vdots & & \\ \frac{\partial f_m}{\partial x_1} & \cdots & \frac{\partial f_m}{\partial x_n} \end{pmatrix}$$

Observe that, by combining the above two steps, if we have a function $f : \mathbb{R}^n \to \mathbb{R}$, then

$$g = \frac{\partial f}{\partial x} \in \mathbb{R}^n \text{ is a vector, with elements } g_i = \frac{\partial f}{\partial x_i}$$
$$H = \frac{\partial g}{\partial x} \in \mathbb{R}^{n \times n} \text{ is a matrix, with elements } H_{ij} = \frac{\partial^2 f}{\partial x_i \partial x_j}.$$

The vector g that contains the first derivative information of f is called the **gradient** of f, and the matrix H that contains the second derivative information of f is called the Hessian of f. There are some "corner cases" (basically having to do with poor continuity properties) where the so-called mixed (or cross partial derivatives) are not equal, but nearly always in machine learning and data science it is the case that

$$\frac{\partial^2 f}{\partial x_i \partial x_j} = \frac{\partial^2 f}{\partial x_j \partial x_i}$$

i.e., that this matrix of second derivatives is symmetric. In this case, everything we have been discussing (e.g., n eigenvalues, a full set of orthonormal eigenvectors, etc.) holds

(e) **Solving eigendecompositions with Lagrange Multipliers.** To compute the eigendecomposition of an $n \times n$ symmetric matrix A, the basic problem in which we are interested is the following. Given a symmetric matrix $A \in \mathbb{R}^{n\times n}$, solve the following constrained optimization problem.

$$\begin{aligned} &\min_{x\in\mathbb{R}^n} x^T A x \\ &\text{subject to} \quad x^T x = 1. \end{aligned} \tag{4}$$

To solve this, we will consider the Lagrangian $L : \mathbb{R}^n \times \mathbb{R} \to R$, defined as follows:

$$L = L(x, \lambda) = x^T A x - \lambda(x^T x - 1),$$

and we will try to solve the following unconstrained optimization problem:

$$\min_{x\in\mathbb{R}^n,\lambda\in\mathbb{R}} (x^T A x - \lambda(x^T x - 1))$$

To do this, consider the first partial derivatives:

$$\begin{aligned} \frac{\partial L}{\partial x} &= 2Ax - 2\lambda x = 0 \\ \frac{\partial L}{\partial \lambda} &= x^T x - 1 = 0. \end{aligned}$$

From the first of these, we have

$$Ax = \lambda x,$$

i.e., we have the equation for eigenvalues and eigenvectors of a matrix; and from the second of these we have

$$x^T x = 1,$$

i.e., that that eigenvector should be normalized. These are very important results. They say that we can recover the expressions for eigenvalues and eigenvectors by considering quadratic functions, which in many ways are simpler to think about. Basically, we have unit circles as input and ellipses as output, and we want to determine the direction of maximum variance in the ellipse, since that corresponds with the vector that maximizes the quadratic form over the unit sphere.

3.3 EVD and Optimization

The requirement that a vector x in $\mathbb{R}^n$ be a unit vector can be stated in several equivalent ways:

$$x^T x = 1, \quad \|x\|^2 = 1, \quad \|x\| = 1$$

and

$$x_1^2 + x_2^2 + \cdots + x_n^2 = 1.$$

When a quadratic form Q has no cross-product terms, it is easy to find the maximum and minimum of $Q(x)$ for $x^T x = 1$.

Example 3.

> Find the maximum and minimum values of $Q(x) = 9x_1^2 + 4x_2^2 + 3x_3^2$ subject to the constraint $x^T x = 1$.

Solution. Since x_2^2 and x_3^2 are nonnegative, note that

$$4x_2^2 \leq 9x_2^2, \quad 3x_3^2 \leq 9x_3^2.$$

We have

$$\begin{aligned} Q(x) &= 9x_1^2 + 4x_2^2 + 3x_3^2 \\ &\le 9x_1^2 + 9x_2^2 + 9x_3^2 \\ &= 9(x_1^2 + x_2^2 + x_3^2) \\ &= 9, \end{aligned}$$

whenever $x_1^2 + x_2^2 + x_3^2 = x^T x = 1$. So the maximum value of $Q(x)$ cannot exceed 9 when x is a unit vector. Furthermore, $Q(x) = 9$ when $x = (1, 0, 0)$. Thus, 9 is the maximum value of $Q(x)$ for $x^T x = 1$.

To find the minimum value of $Q(x)$, observe that

$$9x_1^2 \ge 3x_1^2, \quad 4x_2^2 \ge 3x_2^2.$$

and hence

$$Q(x) = 9x_1^2 + 4x_2^2 + 3x_3^2 \ge 3(x_1^2 + x_2^2 + x_3^2) = 3,$$

whenever $x_1^2 + x_2^2 + x_3^2 = x^T x = 1$. Also, $Q(x) = 3$ when $x = (0, 0, 1)$. So, 3 is the minimum value of $Q(x)$ for $x^T x = 1$.

It is easy to see in this example that the matrix of the quadratic form Q has eigenvalues 9, 4, and 3 and that the greatest and least eigenvalues equal, respectively, the (constrained) maximum and minimum of $Q(x)$. The same holds true for any quadratic form.

Theorem 3.1. *Let A be a symmetric matrix, and*

$$m = \min\{x^T Ax : \|x\| = 1\}m, = \max\{x^T Ax : \|x\| = 1\}.$$

Then M is the greatest eigenvalue λ_1 of A and m is the least eigenvalue of A. The value of $x^T Ax$ is M when x is a unit eigenvector u_1 corresponding to M. The value of $x^T Ax$ is m when x is a unit eigenvector corresponding to m.

Proof. Orthogonally diagonalize A as $V\Lambda V^T$. We observe that if $x = Vy$, then

$$x^T A x = y^T \Lambda y$$

and for all y,

$$\|x\| = \|Vy\| = \|y\|,$$

because $V^T V = I$ and

$$\|Vy\| = (Vy)^T (Vy) = y^T V^T V y = y^T y = \|y\|^2.$$

In particular, $\|y\| = 1$ if and only if $\|x\| = 1$. Thus $x^T A x$ and $y^T \Lambda y$ assume the same set of values as x and y range over the set of all unit vectors.

To simplify notation, suppose that A is a 3×3 matrix with eigenvalues $a \geq b \geq c$. Arrange the (eigenvector) columns of V so that $P = (u_1\ u_2\ u_3)$ and

$$\Lambda = \begin{pmatrix} a & 0 & 0 \\ 0 & b & 0 \\ 0 & 0 & c \end{pmatrix}.$$

We have

$$\begin{aligned} y^T \Lambda y &= a y_1^2 + b y_2^2 + c y_3^2 \\ &\leq a y_1^2 + a y_2^2 + a y_3^2 \\ &= a(y_1^2 + y_2^2 + y_3^2) \\ &= \|y\|^2 = a. \end{aligned}$$

Thus $M \leq a$, by definition of M. However, $y^T \Lambda y = a$ when $y = e_1 = (1, 0, 0)$, so in fact $M = a$. Also, the x that corresponds to $y = e_1$ is the eigenvector u_1 of A, because

$$x = Ve_1 = (u_1\ u_2\ u_3) \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} = u_1$$

Thus

$$M = a = e_1^T \Lambda e_1 = u_1^T A u_1,$$

which proves the statement about M. A similar argument shows that m is the least eigenvalue and this value of $x^T Ax$ is attained when

$$x = Ve_3 = u_3.$$

◀

Theorem 3.2. *Let A, λ_1, and u_1 be as in Theorem 6. Then the maximum value of $x^T Ax$ subject to the constraints*

$$x^T x = 1, \quad x^T u_1 = 0$$

is the second greatest eigenvalue,λ_2, and this maximum is attained when x is an eigenvector u_2 corresponding to λ_2.

This theorem can be proved by an argument similar to the one above in which the theorem is reduced to the case where the matrix of the quadratic form is diagonal. The next example gives an idea of the proof for the case of a diagonal matrix.

Example 4.

> Find the maximum value of $Q(x) = 9x_1^2 + 4x_2^2 + 3x_3^2$ subject to the constraint $x^T x = 1$ and $x^T u_1 = 0$, where $u_1 = (1, 0, 0)$. Note that u_1 is a unit eigenvector corresponding to the greatest eigenvalue $\lambda = 9$ of the matrix of the quadratic form.

Solution. If the coordinates of x are x_1, x_2, x_3, then the constraint $x^T u_1 = 0$ means simply that $x_1 = 0$. For such a unit vector, $x_2^2 + x_3^2 = 1$, and

$$\begin{aligned} 9x_1^2 + 4x_2^2 + 3x_3^2 &= 4x_2^2 + 3x_3^2 \\ &\leq 4(x_2^2 + x_3^2) \\ &= 4. \end{aligned}$$

Thus the constrained maximum of the quadratic form does not exceed 4. And this value is attained for $x_1 = (0, 1, 0)$, which is an eigenvector for the second greatest eigenvalue of the matrix of the quadratic form.

The next theorem generalizes Theorem 7 and, together with Theorem 6, gives a useful characterization of all the eigenvalues of A. The proof is omitted.

Theorem 3.3. *Let A be a symmetric $n \times n$ matrix with an orthogonal diagonalization $A = P\Lambda P^{-1}$, where the entries on the diagonal of Λ are arranged so that $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$ and where the columns of P are corresponding unit eigenvectors $u_1, u_2, \cdots, u_n$. Then for $k = 2, \cdot, n$, the maximum value of $x^T Ax$ subject to the constraints*

$$x^T x = 1,\ x^T u_1 = 0, \cdots, x^T u_{k-1} = 0$$

is the eigenvalue λ_k, and this maximum is attained at $x = u_k$.

4 Singular Value Decomposition

Let's now consider the generalization of the spectral theorem to an arbitrary $m \times n$ matrix A.

The singular value decomposition is based on the following property of the ordinary diagonalization that can be imitated for rectangular matrices: The absolute values of the eigenvalues of a symmetric matrix A measure the amounts that A stretches or shrinks certain vectors (the eigenvectors).

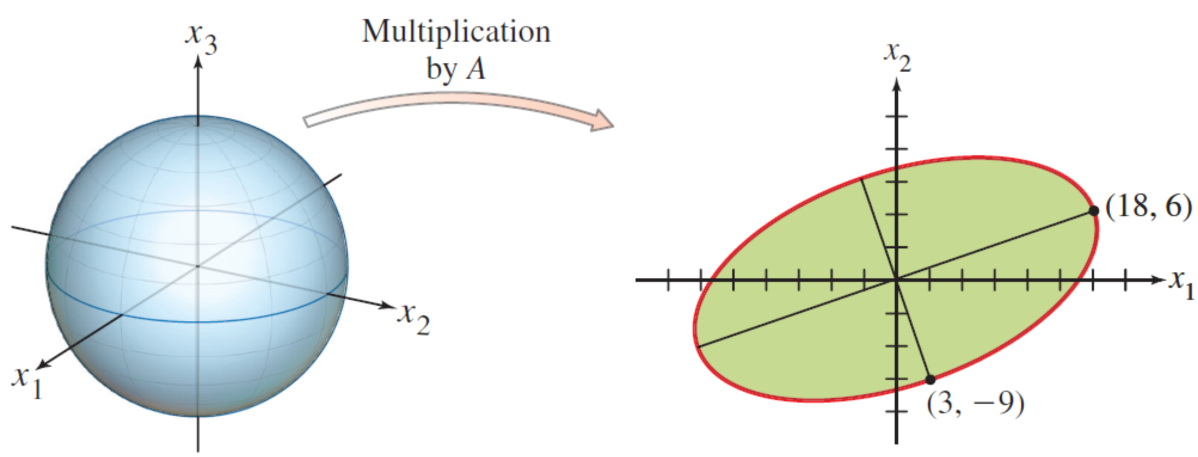
If $Ax = \lambda x$ and $\|x\| = 1$, then

$$\|Ax\| = \|\lambda x\| = |\lambda|\|x\| = |\lambda|.$$

If λ_1 is the largest eigenvalue, then a corresponding unit eigenvector v_1 identifies a direction in which the stretching effect of A is greatest. That is, the length of Ax is maximized when $x = v_1$, and $\|Av_1\| = |\lambda_1|$. This description of v_1 and $|\lambda_1|$ has an analogue for rectangular matrices that will lead to the singular value decomposition.

Example 5.

> If $A = \begin{pmatrix} 4 & 11 & 14 \\ 8 & 7 & -2 \end{pmatrix}$, then the linear transformation $x \mapsto Ax$ maps the unit sphere $\{x : \|x\| = 1\}$ in $\mathbb{R}^3$ onto an ellipse in $\mathbb{R}^2$, shown in the figure. Find a unit vector x at which the length $\|Ax\|$ is maximized, and compute this maximum length.



Solution. The quantity $\|Ax\|^2$ is maximized at the same x that maximizes $\|Ax\|$, and$\|Ax\|^2$ is easier to study. Observe that

$$\|Ax\|^2 = (Ax)^T(Ax) = x^TA^TAx = x^T(A^TA)x.$$

Also, A^TA is a symmetric matrix, since

$$(A^TA)^T = A^TA^{TT} = A^TA.$$

So the problem now is to maximize the quadratic form $x^T(A^TA)x$ subject to the constraint $\|x\| = 1$. We know that the maximum value is the greatest eigenvalue λ_1 of A^TA. Also, the maximum value is attained at a unit eigenvector of A^TA corresponding to λ_1.

For the matrix A in this example,

$$A^TA = \begin{pmatrix} 4 & 8 \\ 11 & 7 \\ 14 & -2 \end{pmatrix} \begin{pmatrix} 4 & 11 & 14 \\ 8 & 7 & -2 \end{pmatrix} = \begin{pmatrix} 80 & 100 & 40 \\ 100 & 170 & 140 \\ 40 & 140 & 200 \end{pmatrix}.$$

The eigenvalues of A^TA are

$$\lambda_1 = 360, \lambda_2 = 90, \lambda_3 = 0.$$

Corresponding unit eigenvectors are, respectively,

$$v_1 = \begin{pmatrix} 1/3 \\ 2/3 \\ 2/3 \end{pmatrix}, v_2 = \begin{pmatrix} -2/3 \\ -1/3 \\ 2/3 \end{pmatrix}, v_3 = \begin{pmatrix} 2/3 \\ -2/3 \\ 1/3 \end{pmatrix}.$$

The maximum value of $\|Ax\|^2$ is 360, attained when x is the unit vector v_1. The vector Av_1 is a point on the ellipse in the above figure farthest from the origin, namely,

$$Av_1 = \begin{pmatrix} 4 & 11 & 14 \\ 8 & 7 & -2 \end{pmatrix} \begin{pmatrix} 1/3 \\ 2/3 \\ 2/3 \end{pmatrix} = \begin{pmatrix} 18 \\ 6 \end{pmatrix}.$$

Therefore, for $\|x\| = 1$, the maximum value of $\|Ax\|$ is

$$\|Av_1\| = \sqrt{360} = 6\sqrt{10}.$$

This example suggests that

- The effect of A on the unit sphere in $\mathbb{R}^3$ is related to the quadratic form $x^T(A^TA)x$.
- To decompose an $m \times n$, it is worthwhile to study A^TA or AA^T. Both are symmetric square matrices and can be orthogonally diagonalized, as we know.

4.1 The Singular Values of an $m \times n$ Matrix

Let A be an $m \times n$ matrix. Then A^TA is symmetric and can be orthogonally diagonalized. Let $\{v_1, \cdots, v_n\}$ be an orthonormal basis for $\mathbb{R}^n$ consisting of eigenvectors of A^TA, and let $\lambda_1, ..., \lambda_n$ be the associated eigenvalues of A^TA. Then, for $1 \le i \le n$,

$$\begin{aligned} \|Av_i\|^2 &= (Av_i)^T Av_i = v_i^T A^T Av_i \\ &= v_i^T(\lambda_i v_i) = \lambda_i(v_i^T v_i) \\ &= \lambda_i \end{aligned}$$

So the eigenvalues of A^TA are all nonnegative. By renumbering, if necessary, we may assume that the eigenvalues are arranged so that

$$\lambda_1 \ge ... \ge \lambda_n \ge 0.$$

The singular values of A are the square roots of the eigenvalues of A^TA, denoted by

$$\sigma_1, ..., \sigma_n.$$

and they are arranged in decreasing order. That is,

$$\sigma_i = \sqrt{\lambda_i} \quad 1 \leq i \leq n.$$

Note that the singular values of A are the lengths of the vectors $Av_1, ..., Av_n$.

Example 6.

Let A be the matrix in Example (5). Since the eigenvalues of $A^T A$ are 360, 90, and 0, the singular values of A are

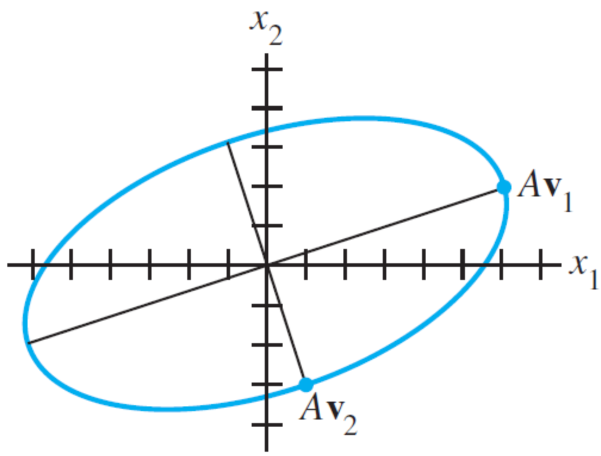
$$\sigma_1 = 6\sqrt{10},\ \sigma_2 = \sqrt{90} = 3\sqrt{10},\ \sigma_3 = 0.$$

From Example 5, the first singular value of A is the maximum of $\|Ax\|$ over all unit vectors, and the maximum is attained at the unit eigenvector v_1. We know that the second singular value of A is the maximum of $\|Ax\|$ over all unit vectors that are orthogonal to v_1, and this maximum is attained at the second unit eigenvector, v_2. For the v_2 in Example 5,

$$Av_2 = \begin{pmatrix} 4 & 11 & 14 \\ 8 & 7 & -2 \end{pmatrix} \begin{pmatrix} -2/3 \\ -1/3 \\ 2/3 \end{pmatrix} = \begin{pmatrix} 3 \\ -9 \end{pmatrix}.$$

This point is on the minor axis of the ellipse in the figure given in Example 5, just as Av_1 is on the major axis. (See the figure below.) The first two singular values of A are the lengths of the major and minor semiaxes of the ellipse.

The fact that Av_1 and Av_2 are orthogonal in the above figure is no accident, as the next theorem shows.



Theorem 4.1. *Suppose $\{v_1, \cdots, v_n\}$ is an orthonormal basis of $\mathbb{R}^n$ consisting of eigenvectors of A^TA, arranged so that the corresponding eigenvalues of A^TA satisfy $\lambda_1 \geq ... \geq \lambda_n$, and suppose A has r nonzero singular values. Then $\{Av_1, \cdots, Av_n\}$ is an orthogonal basis for* Col A*, and* rank $A = r$.

Proof. Because v_i and $\lambda_j v_j$ are orthogonal for $i \neq j$,

$$(Av_i)^T Av_i = v_i^T A^T Av_i = v_i^T(\lambda_i v_i) = 0$$

Thus $\{Av_1, \cdots, Av_n\}$ is an orthogonal set. Furthermore, since the lengths of the vectors $Av_1, \cdots, Av_n$ are the singular values of A, and since there are r nonzero singular values,

$$Av_i \neq 0 \Leftrightarrow 1 \leq i \leq r.$$

So $Av_1, \cdots, Av_r$ are linearly independent vectors, and they are in Col A. Finally, for any y in Col A, say, $y = Ax$, we can write

$$x = c_1 v_1 + \cdots + c_n v_n,$$

and

$$\begin{aligned} y = Ax &= c_1 Av_1 + \cdots + c_r Av_r + \cdots + c_n Av_n \\ &= c_1 Av_1 + \cdots + c_r Av_r + 0 + \cdots + 0. \end{aligned}$$

Thus, y is in span $(Av_1, \cdots, Av_r)$, which shows that $\{Av_1, \cdots, Av_r\}$ is an (orthogonal) basis for Col A. Hence

$$\operatorname{rank} A = \dim \operatorname{Col} A = r. \qquad \blacktriangleleft$$

4.2 The Singular Value Decomposition

The decomposition of A involves an $m \times n$ "diagonal" matrix Σ of the form where D is an $r \times r$ diagonal matrix for some r not

$$\Sigma = \begin{array}{cl} \begin{bmatrix} D & 0 \\ 0 & 0 \end{bmatrix} & \begin{array}{l} \\ \leftarrow m - r \text{ rows} \end{array} \\ \qquad\quad \uparrow\ n - r \text{ columns} & \end{array}$$

exceeding the smaller of m and n. (If r equals m or n or both, some or all of the zero matrices do not appear.)

Theorem 4.2. *Let A be an $m \times n$ matrix with rank r. Then there exists an $m \times n$ matrix Σ as in the above for which the diagonal entries in D are the first r singular values of A,*

$$\sigma_1 \geq \cdots \geq \sigma_r > 0$$

and there exist an $m \times m$ orthogonal matrix U and an $n \times n$ orthogonal matrix V such that

$$A = U \Sigma V^T.$$

Any factorization $A = U\Sigma V^T$, with U and V orthogonal, Σ as in the above, and positive diagonal entries in D, is called a **singular value decomposition** (or SVD) of A. The matrices U and V are not uniquely determined by A, but the diagonal entries of Σ are necessarily the singular values of A. The columns of U in such a decomposition are called **left singular vectors** of A, and the columns of V are called **right singular vectors** of A.

Example 7.

Use the results of Examples 5 and 6 to construct a singular value decomposition of $A = \begin{pmatrix} 4 & 11 & 14 \\ 8 & 7 & -2 \end{pmatrix}$.

Solution. A construction can be divided into three steps.

Step 1. Find an orthogonal diagonalization of $A^T A$.
That is, find the eigenvalues of $A^T A$ and a corresponding orthonormal set of eigenvectors. If A had only two columns, the calculations could be done by hand. Larger matrices usually require a matrix program. However, for the matrix A here, the eigendata for $A^T A$ are provided in Example 5.

Step 2. Set up V and Σ. Arrange the eigenvalues of $A^T A$ in decreasing order. In Example 5, the eigenvalues are already listed in decreasing order: 360, 90, and 0. The corresponding unit eigenvectors, v_1, v_2, and v_3, are the right singular vectors of A. Using Example 5, construct

$$V = (v_1 \; v_2 \; v_3) = \begin{pmatrix} 1/3 & -2/3 & 2/3 \\ 2/3 & -1/3 & -2/3 \\ 2/3 & 2/3 & 1/3 \end{pmatrix}.$$

The square roots of the eigenvalues are the singular values:

$$\sigma_1 = 6\sqrt{10},\ \sigma_2 = \sqrt{90} = 3\sqrt{10},\ \sigma_3 = 0.$$

The nonzero singular values are the diagonal entries of D. The matrix Σ is the same size as A, with D in its upper left corner and with 0s elsewhere.

$$D = \begin{pmatrix} 6\sqrt{10} & 0 \\ 0 & 3\sqrt{10} \end{pmatrix},\ \Sigma = (D\, 0) = \begin{pmatrix} 6\sqrt{10} & 0 & 0 \\ 0 & 3\sqrt{10} & 0 \end{pmatrix}.$$

Step 3. Construct U. When A has rank r, the first r columns of U are the normalized vectors obtained from $Av_1, \cdots, Av_n$. In this example, A has two nonzero singular values, so rank $A = 2$. We know that

$$\|Av_1\| = \sigma_1, \quad \|Av_2\| = \sigma_2.$$

Thus,

$$u_1 = \frac{1}{\sigma_1} Av_1 = \frac{1}{6\sqrt{10}} \begin{pmatrix} 18 \\ 6 \end{pmatrix} = \begin{pmatrix} 3\sqrt{10} \\ 1\sqrt{10} \end{pmatrix}.$$

and

$$u_2 = \frac{1}{\sigma_2} Av_2 = \frac{1}{3\sqrt{10}} \begin{pmatrix} 3 \\ -9 \end{pmatrix} = \begin{pmatrix} 1\sqrt{10} \\ -3/\sqrt{10} \end{pmatrix}.$$

Note that $\{u_1, u_2\}$ is already a basis for $\mathbb{R}^2$. Thus no additional vectors are needed for U, and $U = (u_1\ u_2)$. The singular value decomposition of A is

$$A = \begin{pmatrix} 3\sqrt{10} & 1\sqrt{10} \\ 1\sqrt{10} & -3/\sqrt{10} \end{pmatrix} \begin{pmatrix} 6\sqrt{10} & 0 & 0 \\ 0 & 3\sqrt{10} & 0 \end{pmatrix} \begin{pmatrix} 1/3 & -2/3 & 2/3 \\ 2/3 & -1/3 & -2/3 \\ 2/3 & 2/3 & 1/3 \end{pmatrix}.$$

4.3 Equivalent ways to view the SVD

4.4 SVD and thin SVD and rank-deficient thin SVD

5 Additional properties of the SVD

5.1 SVD and the structure of $\mathbb{R}^m$ and $\mathbb{R}^n$

5.2 SVD and the norm of a matrix

5.3 SVD and inverses of non-invertible matrices: the pseudoinverse