1 Last time: symmetric matrices

A matrix A is symmetric if $A^T = A$.

This happens if and only if A is square and $A_{ij} = A_{ji}$ for all i, j.

Example.
$$\begin{bmatrix} 1 & 2 \\ 2 & 3 \end{bmatrix}$$
 is symmetric but $\begin{bmatrix} 1 & 2 \\ 3 & 2 \end{bmatrix}$ is not.

A matrix U is orthogonal if U is invertible and $U^{-1} = U^T$.

This happens precisely when U is square with orthonormal columns.

An $n \times n$ matrix A is orthogonally diagonalisable if there is an orthogonal matrix U and a diagonal matrix D such that $A = UDU^{-1} = UDU^{T}$. In this case, the columns of U are an orthonormal basis for \mathbb{R}^{n} consisting of eigenvectors for A, and the eigenvalues of these eigenvectors are the diagonal entries of D.

The following summarises the main results from last time:

Theorem.

- (1) A square matrix is orthogonally diagonalisable if and only if it is symmetric.
- (2) Eigenvectors with distinct eigenvalues of a symmetric matrix are orthogonal.
- (3) All (complex) eigenvalues of a symmetric matrix A are real, i.e., the characteristic polynomial of A has all real roots and can be expressed as $\det(A xI) = (\lambda_1 x)(\lambda_2 x)\cdots(\lambda_n x)$ for some not-necessarily-distinct real numbers $\lambda_1, \lambda_2, \ldots, \lambda_n \in \mathbb{R}$.

Example. Suppose
$$A = \begin{bmatrix} a & b \\ b & a \end{bmatrix}$$
 for some $a, b \in \mathbb{R}$.

How does the preceding theorem apply to this generic 2-by-2 matrix? Since

$$\det(A - xI) = \det \begin{bmatrix} a - x & b \\ b & a - x \end{bmatrix} = (a - x)^2 - b^2 = (a - b - x)(a + b - x),$$

the eigenvalues of A are a - b and a + b.

It's not too hard to guess the eigenvectors corresponding to these eigenvectors just by looking, though the usual method of finding eigenvectors by row reducing $A - \lambda I$ to find a basis for $\operatorname{Nul}(A - \lambda I)$ will also produce the answer.

Namely, the vector $\left[\begin{array}{c} 1 \\ -1 \end{array}\right]$ is an eigenvector for A with eigenvalue a-b.

The vector $\begin{bmatrix} 1 \\ 1 \end{bmatrix}$ is an eigenvector for A with eigenvalue a + b.

These eigenvectors are orthogonal, as predicted by the theorem. We can convert them to unit vectors by multiplying each vector by the reciprocal of its length. This gives the eigenvectors

$$\begin{bmatrix} 1\sqrt{2} \\ -1/\sqrt{2} \end{bmatrix} \quad \text{and} \quad \begin{bmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \end{bmatrix}$$

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which form an orthonormal basis for \mathbb{R}^2 .

It follows that
$$A = UDU^{-1} = UDU^T$$
 where $U = \begin{bmatrix} 1\sqrt{2} & 1/\sqrt{2} \\ -1/\sqrt{2} & 1/\sqrt{2} \end{bmatrix}$ and $D = \begin{bmatrix} a-b & 0 \\ 0 & a+b \end{bmatrix}$.

2 Singular value decomposition

Today, we'll apply the results from last time to prove the existence of *singular value decompositions*, which will give a sort of approximate orthogonal diagonalisation for any matrix, not just symmetric ones.

Let A be an $m \times n$ matrix.

Then $A^T A$ is a symmetric $n \times n$ matrix, since $(A^T A)^T = A^T (A^T)^T = A^T A$.

It follows from our results last time that A^TA has all real eigenvalues. A stronger statement holds:

Lemma. All eigenvalues of A^TA are nonnegative real numbers.

Proof. Since A^TA is symmetric, we know that the matrix can be orthogonally diagonalised. In other words, we know there exists an orthonormal basis v_1, v_2, \ldots, v_n for \mathbb{R}^n consisting of eigenvectors of A^TA . Let $\lambda_1, \lambda_2, \ldots, \lambda_n \in \mathbb{R}$ be the associated eigenvalues, so that $A^TAv_i = \lambda_i v_i$ for $i = 1, 2, \ldots, n$. Then

$$||Av_i||^2 = (Av_i) \bullet (Av_i) = (Av_i)^T (Av_i) = v_i^T A^T Av_i = v_i^T (\lambda_i v_i) = \lambda_i ||v_i||^2 = \lambda_i$$

for each index i. Since $||Av_i|| \ge 0$, it follows that every eigenvalue satisfies $\lambda_i \ge 0$.

The preceding lemma allows us to make the following definition.

Definition. Let $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n \geq 0$ be the eigenvalues of $A^T A$ arranged in decreasing order. Define $\sigma_i = \sqrt{\lambda_i}$ for $i = 1, 2, \dots, n$. We call the numbers $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_n \geq 0$ the singular values of A.

In other words, the singular values of a matrix A are the squares roots of the eigenvalues of $A^T A$, which are guaranteed to be nonnegative real numbers (and therefore always have well-defined square roots).

Example. Suppose
$$A = \begin{bmatrix} 4 & 11 & 14 \\ 8 & 7 & -2 \end{bmatrix}$$
. Then $A^T A = \begin{bmatrix} 80 & 100 & 40 \\ 100 & 170 & 140 \\ 40 & 140 & 200 \end{bmatrix}$.

This matrix $A^T A$ has characteristic polynomial

$$\det(A^T A - xI) = (360 - x)(90 - x)x$$

so the eigenvalues of A^TA are $\lambda_1 = 360$, $\lambda_2 = 90$, and $\lambda_3 = 0$.

The singular values of A are therefore $\sigma_1 = \sqrt{360}$, $\sigma_2 = \sqrt{90}$, and $\sigma_3 = 0$.

As a sequel to the lemma above, we have this nontrivial statement about the eigenvectors of $A^{T}A$.

Theorem. Suppose v_1, v_2, \ldots, v_n is an orthonormal basis of \mathbb{R}^n composed of eigenvectors of $A^T A$, arranged so that if $\lambda_i \in \mathbb{R}$ is the eigenvalue of v_i then $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$.

Assume A has r nonzero singular values.

Then Av_1, Av_2, \ldots, Av_r is an orthogonal basis for the column space of A and consequently rank A = r.

Proof. Choose indices $i \neq j$. Then $v_i \bullet v_j = 0$ so also $v_i \bullet \lambda_i v_j = 0$.

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

This shows that Av_1, Av_2, \ldots, Av_r are orthogonal vectors in Col A.

Since $||Av_i|| = \sqrt{\lambda_i} > 0$, these vectors are all nonzero and therefore are linearly independent.

To see that these vectors span the column space of A, suppose $y \in \text{Col } A$. The y = Ax for some vector $x \in \mathbb{R}^n$, which we can write as $x = c_1v_1 + c_2v_2 + \cdots + c_nv_n$ for some coefficients $c_1, c_2, \ldots, c_n \in \mathbb{R}$. Then

$$y = Ax = c_1 A v_1 + c_2 A v_2 + \dots + c_r A v_r + \underbrace{c_{r+1} A v_{r+1} + \dots + c_n A v_n}_{=0} = c_1 A v_1 + c_2 A v_2 + \dots + c_r A v_r$$

since $Av_i = 0$ as $||Av_i|| = \sqrt{\lambda_i} = 0$ for i > r. We conclude that Av_1, Av_2, \dots, Av_r is a basis for Col A. \square

Corollary. The rank of a matrix is the same as its number of nonzero singular values.

We arrive at today's main result.

Theorem (Existence of SVDs). Let A be an $m \times n$ matrix with rank r. Then we can write

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

where

- (i) U is some $m \times m$ orthogonal matrix.
- (ii) V is some $n \times n$ orthogonal matrix.
- (iii) Σ is the $m \times n$ matrix

$$\Sigma = \left[egin{array}{ccc} D & 0 \\ 0 & 0 \end{array}
ight] \qquad ext{where } D = \left[egin{array}{ccc} \sigma_1 & & & \\ & \sigma_2 & & \\ & & \ddots & \\ & & & \sigma_r \end{array}
ight]$$

and $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_r$ are the singular values of A.

Comments. The three zeros in the matrix defining Σ are implicitly blocks of zeros: the upper right 0 stands for an $r \times (n-r)$ zero submatrix, the lower right 0 stands for an $(m-r) \times (n-r)$ zero submatrix, and the lower left 0 stands for an $(m-r) \times r$ zero submatrix.

Another way to think of Σ : place the diagonal matrix D in the upper left corner of an $m \times n$ matrix, and then fill all of the remaining entries with zeros.

A factorisation $A = U\Sigma V^T$ with U, V, and Σ as in (i)-(iii) is a singular value decomposition (SVD) of A.

The matrices U and V in an SVD $A = U\Sigma V^T$ are not uniquely determined by A, but Σ is. The columns of U are the *left singular vectors* of A while the columns of V are the *right singular vectors* of A.

Proof that an SVD of A exists. Let $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$ be the decreasing list of eigenvalues of $A^T A$.

Let v_1, v_2, \ldots, v_n a list of corresponding orthonormal eigenvectors for $A^T A$.

Then $\lambda_{r+1} = \lambda_{r+2} = \cdots = \lambda_n = 0$ are Av_1, Av_2, \ldots, Av_r is an orthogonal basis for Col A.

For each $i = 1, 2, \ldots, r$, define

$$u_i = \frac{1}{\|Av_i\|} Av_i = \frac{1}{\sqrt{\lambda_i}} Av = \frac{1}{\sigma_i} Av_i.$$

Then u_1, u_2, \ldots, u_r is an orthonormal basis for Col A.

We can choose vectors $u_{r+1}, u_{r+2}, \dots, u_m \in \mathbb{R}^m$ such that the extended list of vectors u_1, u_2, \dots, u_m is an orthonormal basis for \mathbb{R}^m . Make any such choice, and define

$$U = [u_1 \quad u_2 \quad \dots \quad u_m]$$
 and $V = [v_1 \quad v_2 \quad \dots \quad v_n].$

These matrices are orthogonal by construction, and

$$AV = \begin{bmatrix} Av_1 & Av_2 & \dots & Av_n \end{bmatrix}$$

=
$$\begin{bmatrix} Av_1 & Av_2 & \dots & Av_r & 0 & \dots & 0 \end{bmatrix} = \begin{bmatrix} \sigma_1 u_1 & \sigma_2 u_2 & \dots & \sigma_r u_r & 0 & \dots & 0 \end{bmatrix}.$$

If Σ is the matrix given in (iii), then we also have

$$U\Sigma = \begin{bmatrix} \sigma_1 u_1 & \sigma_2 u_2 & \dots & \sigma_r u_r & 0 & \dots & 0 \end{bmatrix} = AV$$

so $U\Sigma V^T = AVV^T = AI = A$, which confirms the theorem statement.

We conclude this lecture with a small example, continuing from before.

Example. Again suppose $A = \begin{bmatrix} 4 & 11 & 14 \\ 8 & 7 & -2 \end{bmatrix}$.

To find a singular value decomposition for A, there are three steps.

1. Find an orthogonal diagonalisation of A^TA .

In this case A^TA is a 3×3 matrix, and by the usual methods (of row reducing $A - \lambda I$ to find a basis for $\text{Nul}(A - \lambda I)$ for each eigenvalue λ), you can find that

$$v_1 = \begin{bmatrix} 1/3 \\ 2/3 \\ 2/3 \end{bmatrix}, \quad v_2 = \begin{bmatrix} -2/3 \\ -1/3 \\ 2/3 \end{bmatrix}, \quad \text{and} \quad v_3 = \begin{bmatrix} 2/3 \\ -2/3 \\ 1/3 \end{bmatrix}$$

is an orthonormal basis of \mathbb{R}^3 consisting of eigenvectors of A^TA , with corresponding eigenvalues $\lambda_1 = 360$, $\lambda_2 = 90$, and $\lambda_3 = 0$.

2. Set up V and Σ .

Following the proof of the theorem, we have

$$V = \begin{bmatrix} v_1 & v_2 & v_3 \end{bmatrix} = \frac{1}{3} \begin{bmatrix} 1 & -2 & 2 \\ 2 & -1 & -2 \\ 2 & 2 & 1 \end{bmatrix} \quad \text{and} \quad D = \begin{bmatrix} \sigma_1 & 0 \\ 0 & \sigma_2 \end{bmatrix}$$

for $\sigma_1 = \sqrt{\lambda_1} = \sqrt{360}$ and $\sigma_2 = \sqrt{\lambda_2} = \sqrt{90}$.

Since Σ must have the same size as A, we get

$$\Sigma = \left[\begin{array}{cc} \sqrt{360} & 0 & 0 \\ 0 & \sqrt{90} & 0 \end{array} \right].$$

3. Construct U.

We have $U = \begin{bmatrix} u_1 & u_2 \end{bmatrix}$ where $u_i = \frac{1}{\sigma_i} A v_i$.

In this case you can compute that

$$u_1 = \frac{1}{\sqrt{360}} \begin{bmatrix} 18 \\ 6 \end{bmatrix}$$
 and $u_2 = \frac{1}{\sqrt{90}} \begin{bmatrix} 3 \\ -9 \end{bmatrix}$

which means that we can write

$$U = \frac{1}{\sqrt{10}} \left[\begin{array}{cc} 3 & -1 \\ 1 & -3 \end{array} \right].$$

Putting everything together produces the singular value decomposition

$$A = U\Sigma V^T = \begin{bmatrix} 3/\sqrt{10} & 1/\sqrt{10} \\ 1/\sqrt{10} & -3/\sqrt{10} \end{bmatrix} \begin{bmatrix} \sqrt{360} & 0 & 0 \\ 0 & \sqrt{90} & 0 \end{bmatrix} \begin{bmatrix} 1/3 & 2/3 & 2/3 \\ -2/3 & -1/3 & 2/3 \\ 2/3 & -2/3 & 1/3 \end{bmatrix}.$$

Be careful to note that the third matrix factor is the transpose V^T rather than V.