Singular Value Decomposition

Abhinav Anand, IIMB

2023/01/31

Eigendecomposition

Before learning what is singular value decomposition, it will be useful to remind ourselves what is eigendecomposition.

A vector $v_{n \times 1}$ is an eigenvector to a (square) matrix $A_{n \times n}$ if applying it to A (postmultiplying it) results in getting back the vector v, with some scaling $\lambda_{1 \times 1}$.

$$A_{n \times n} v_{n \times 1} = \lambda_{1 \times 1} v_{n \times 1}$$

Clearly, if $\lambda > 0$, the application of v on A produces an expansion in the direction of v, else a contraction.

A particularly simple way to geometrically interpret the eigenvector is that it is a *fixed direction* which is unchanged by the matrix A.

In general, a square matrix acts on some domain and transforms it into some image. However (under some mild conditions) it turns out that for each such matrix A whose domain is the n dimensional linear space $\mathbb{R}^n$, there are exactly n fixed directions $v_1, v_2, \ldots, v_n$, or in other words, points on the fixed directions v_i remain fixed under the application of the matrix A and can only be sent 'outwards' (if $\lambda_i > 0$) corresponding to an 'expansion', or be sent 'inwards' (if $\lambda_i < 0$) corresponding to a 'contraction'. Even further, these fixed directions can form a basis for the domain and the image spaces. Note that this is far from obvious. (Indeed why should there be any fixed directions?)

1

Moreover, a simple transformation gives more insights about these eigenvectors:

$$(A_{n\times n} - \lambda I_{n\times n})v_{n\times 1} = 0_{n\times 1}$$

The above equation indicates that the eigenvector v is in fact a resident of the *null space* (or *kernel*) of $A - \lambda I$.

Continuing on with the definition of eigenvectors, we note that for a generic $A_{n\times n}$ matrix, there are n eigenvectors $v_1, \ldots, v_n$ which form the basis of the domain $\mathbb{R}^n$. Thus for each such vector, applying the definition, we get:

$$Av_1 = \lambda_1 v_1$$
$$Av_2 = \lambda_2 v_2$$
$$\vdots$$
$$Av_n = \lambda_n v_n$$

Denoting the above operations in matrix form, we get

$$A_{n\times n}[v1_{n\times 1}, v2_{n\times 1}, \ldots, vn_{n\times 1}] = [v1_{n\times 1}, v2_{n\times 1}, \ldots, vn_{n\times 1}]\begin{bmatrix} \lambda_1 & & \\ & \ddots & \\ & & \lambda_n \end{bmatrix}$$

Or in more compact notation

$$A_{n\times n}Q_{n\times n} = \Lambda_{n\times n}Q_{n\times n}$$
$$A = Q\Lambda Q^{-1}$$

This is the famous eigendecomposition of a matrix into its eigenvector matrix Q and the diagonal eigenvalue matrix Λ.

Another way to interpret the same equation is the following:

$$\because A = Q\Lambda Q^{-1} \Rightarrow Q^{-1}AQ = \Lambda$$

This, in plain language, denotes that any square matrix is decomposable into a diagonal matrix whose entries are its eigenvalues.

The above can be refined even further if the matrix under consideration is symmetric. In that case, the eigenvalues are real. Further, if the matrix is positive definite the eigenvalues are positive, and if it is negative definite, the eigenvalues are negative. For the symmetric positive definite matrix, an added feature is that the eigenvectors are orthogonal to each other, and in fact, the inverse of the eigenmatrix is simply its transpose, i.e., $Q^{-1} = Q^{\top}$.

$$A = Q \Lambda Q^{\top}$$

This will be our starting point for understanding the singular value decomposition.

Singular Value Decomposition (SVD)

The best part about SVD is that it is applicable not just to square matrices, but in fact to *any* matrix $A_{m \times n}$:

$$A_{m \times n} = \underbrace{U_{m \times m}}_{orthogonal} \overbrace{\Sigma_{m \times n}}^{diagonal} \underbrace{V_{n \times n}^{\top}}_{orthogonal}$$

The middle matrix $\Sigma_{m \times n}$ is a diagonal matrix whose entries are positive, and are called 'singular values' of A, denoted by $\sigma_1, \ldots, \sigma_r$. They fill out the first r entries of the diagonal matrix, assuming A has rank $r < min(m, n)$. Interestingly, the singular values are in fact, the square roots of eigenvalues of $A^{\top}A$.

Let's interpret the SVD components one by one:

Left-singular matrix: $U_{m \times m}$

The columns of U form the eigenvectors of $AA^{\top}$. We can see this clearly below:

$$AA^{\top} = (U\Sigma V^{\top})(V\Sigma^{\top}U^{\top}) = U\Sigma \underbrace{V^{\top}V}_{=I_{n \times n}} \Sigma^{\top}U^{\top} = U\underbrace{\Sigma\Sigma^{\top}}_{\widetilde{\Sigma}}U^{\top} = U\widetilde{\Sigma}U^{\top}$$

Or, in other words, U must be the eigenmatrix for $AA^\top$. The matrix in the middle: $\Sigma\Sigma^\top$ is $m \times m$ and carries the entries $\sigma_1^2, \ldots, \sigma_r^2$ on the diagonal.

Right-singular matrix: $V_{n \times n}^\top$

The columns of V form the eigenvectors of $A^\top A$.

$$A^\top A = (U\Sigma V^\top)^\top (U\Sigma V^\top) = V\Sigma^\top \underbrace{U^\top U}_{=I_{m \times m}} \Sigma V^\top = V \underbrace{\Sigma^\top \Sigma}_{\widehat{\Sigma}} V^\top = V\widehat{\Sigma} V^\top$$

Or, in other words, V must be the eigenmatrix for $A^\top A$. The matrix in the middle: $\Sigma^\top \Sigma$ is $n \times n$ and carries the entries $\sigma_1^2, \ldots, \sigma_r^2$ on the diagonal.

Relation with the four fundamental subspaces

U and V give orthonormal bases for all the four fundamental subspaces of the matrix A

1. The first r columns of U form the basis of the *column space* of A
2. The last $m - r$ columns of U form the basis of the *left nullspace* of A
3. The first r columns of V form the basis of the *row space* of A
4. The last $m - r$ columns of V form the basis of the *nullspace* of A

Operational interpretation

Another way to look at the singular-value decomposition is in terms of the following operation

$$A_{m \times n}(v_i)_{n \times 1} = \sigma_i(u_i)_{m \times 1}$$

$$A_{m \times n}[(v_1)_{n \times 1}, \ldots, (v_n)_{n \times 1}] = [(u_1)_{m \times 1}, \ldots, (u_m)_{n \times 1}] \begin{bmatrix} \sigma_1 & & & & \\ & \ddots & & & \\ & & \sigma_n & & \\ & & & \ddots & \\ & & & & 0 \end{bmatrix}$$

4

$$AV = U\Sigma$$

Applications: Principal components

Applications: Least squares regressions