

Singular Value Decomposition (SVD) tutorial

BE.400 / 7.548

Singular value decomposition takes a rectangular matrix of gene expression data (defined as A , p matrix) in which the n rows represents the genes, and the p columns represents the experimenter. The SVD theorem states:

$$A_{n \times p} = U_{n \times n} S_{n \times p} V_{p \times p}^T$$

Where

$$U^T U = I_{n \times n}$$

$$V^T V = I_{p \times p} \text{ (i.e. } U \text{ and } V \text{ are orthogonal)}$$

Where the columns of U are the left singular vectors (*gene coefficient vectors*); S (the same dimension as A) contains singular values and is diagonal (*mode amplitudes*); and V^T has rows that are the right singular vectors (*expression level vectors*). The SVD represents an expansion of the original data in a coordinate system where the covariance matrix is diagonal.

Calculating the SVD consists of finding the eigenvalues and eigenvectors of AA^T and $A^T A$. The eigenvectors of $A^T A$ make up the columns of V , the eigenvectors of AA^T make up the columns of U . Also, the singular values are the square roots of eigenvalues from AA^T or $A^T A$. The singular values are the diagonal entries of S and are arranged in descending order. The singular values are always real numbers. If the matrix A is real, then U and V are also real.

To understand how to solve for SVD, let's take the example of the matrix that was provided in

$$A = \begin{bmatrix} 2 & 4 \\ 1 & 3 \\ 0 & 0 \\ 0 & 0 \end{bmatrix}$$

In this example the matrix is a 4x2 matrix. We know that for an $n \times n$ matrix W , then a nonzero eigenvector of W if:

$$W \mathbf{x} = \lambda \mathbf{x}$$

For some scalar λ . Then the scalar λ is called an eigenvalue of A , and \mathbf{x} is said to be an eigenvector corresponding to λ .

So to find the eigenvalues of the above entity we compute matrices AA^T and $A^T A$. As previous eigenvectors of AA^T make up the columns of U so we can do the following analysis to find U .

Now that we have a $n \times n$ matrix we can determine the eigenvalues of the matrix W .

$$\text{Since } W \mathbf{x} = \lambda \mathbf{x} \text{ then } (W - \lambda I) \mathbf{x} = 0$$

$$\begin{bmatrix} 20 - \lambda & 14 & 0 & 0 \\ 14 & 10 - \lambda & 0 & 0 \\ 0 & 0 & -\lambda & 0 \\ 0 & 0 & 0 & -\lambda \end{bmatrix} \mathbf{x} = (W - \lambda I) \mathbf{x} = 0$$

For a unique set of eigenvalues to determinant of the matrix $(W - \lambda I)$ must be equal to zero. solution of the characteristic equation, $|W - \lambda I| = 0$ we obtain:

$\lambda = 0, \lambda = 0; \lambda = 15 + \sqrt{221.5} \sim 29.883; \lambda = 15 - \sqrt{221.5} \sim 0.117$ (four eigenvalues since it is a four polynomial). This value can be used to determine the eigenvector that can be placed in the columns we obtain the following equations:

$$19.883 x_1 + 14 x_2 = 0$$

$$14 x_1 + 9.883 x_2 = 0$$

$$x_3 = 0$$

$$x_4 = 0$$

Upon simplifying the first two equations we obtain a ratio which relates the value of x_1 to x_2 . and x_2 are chosen such that the elements of the S are the square roots of the eigenvalues. Thus satisfies the above equation $x_1 = -0.58$ and $x_2 = 0.82$ and $x_3 = x_4 = 0$ (this is the second column

Substituting the other eigenvalue we obtain:

$$-9.883 x_1 + 14 x_2 = 0$$

$$14 x_1 - 19.883 x_2 = 0$$

$$x_3 = 0$$

$$x_4 = 0$$

Thus a solution that satisfies this set of equations is $x_1 = 0.82$ and $x_2 = -0.58$ and $x_3 = x_4 = 0$ (the first column of the U matrix). Combining these we obtain:

$$U = \begin{bmatrix} 0.82 & -0.58 & 0 & 0 \\ 0.58 & 0.82 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

Similarly $A^T A$ makes up the columns of V so we can do a similar analysis to find the value of V

$$A^T A = \begin{bmatrix} 2 & 4 & 0 & 0 \\ 1 & 3 & 0 & 0 \end{bmatrix} \begin{bmatrix} 2 & 4 \\ 1 & 3 \\ 0 & 0 \\ 0 & 0 \end{bmatrix}$$

and similarly we obtain the expression:

$$S = \begin{bmatrix} 5.47 & 0 \\ 0 & 0.37 \\ 0 & 0 \\ 0 & 0 \end{bmatrix}$$

Note that: $\sigma_1 > \sigma_2 > \sigma_3 > \dots$ which is what the paper was indicating by the figure 4 of the Kuhlman et al. (2002) paper. In that paper the values were computed and normalized such that the highest singular value was equal to 1.

Proof:

$$\mathbf{A} = \mathbf{U}\mathbf{S}\mathbf{V}^T \text{ and } \mathbf{A}^T = \mathbf{V}\mathbf{S}\mathbf{U}^T$$

$$\mathbf{A}^T \mathbf{A} = \mathbf{V}\mathbf{S}\mathbf{U}^T \mathbf{U}\mathbf{S}\mathbf{V}^T$$

$$\mathbf{A}^T \mathbf{A} = \mathbf{V}\mathbf{S}^2\mathbf{V}^T$$

$$\mathbf{A}^T \mathbf{A}\mathbf{V} = \mathbf{V}\mathbf{S}^2$$

References

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