

CPL Project

Singular Value Decomposition (SVD)

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1 Terminology and Theorem

Given $A \in R^{m \times n}$, there exist orthogonal matrices $U \in R^{m \times m}$ and $V \in R^{n \times n}$, and a diagonal matrix $\Sigma \in R^{m \times n}$ with non-negative diagonal entries such that

$$A_{m \times n} = U_{m \times m} \Sigma_{m \times n} V_{n \times n}^T \quad (1)$$

(if there are complex matrices, transpose can be replaced with complex conjugate) where U, V are unitary matrices. So,

$$U^T U = I_{m \times m} \quad (2)$$

$$V^T V = I_{n \times n} \quad (3)$$

The diagonal entries of Σ are called the singular values of A . The columns of U are called the left singular vectors, and those of V are called the right singular vectors. The singular values are unique, but U and V are not unique.

The number of nonzero singular values is equal to the rank of the matrix A .

2 Theory

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 in S are square roots of eigenvalues from AA^T or $A^T A$. The singular values are the diagonal entries of the S matrix and are arranged in descending order. The singular values are always real numbers. If the matrix A is a real matrix, then U and V are also real. Here, we chose to find V by computing $A^T A$. We use an approximate method to compute eigenvalues of a diagonalizable matrix called the “Power method”.

$$A^T A = (U\Sigma V^T)^T (U\Sigma V^T) = (V\Sigma U^T)(U\Sigma V^T) = V\Sigma^2 V^T \quad (4)$$

So we can completely eliminate U from the discussion, and look at just $V \Sigma^2 V^T$. And what’s nice about this matrix is that we can compute its eigen-vectors, and these turn out to be exactly the singular vectors. The corresponding eigenvalues are the squared singular values. If you apply $(V \Sigma^2 V^T)$ to any v_i (singular vector), the only parts of the product that are non-zero are the ones involving v_i with itself, and the scalar σ_i^2 factors in smoothly.

Call $V\Sigma^2 V^T = B$. Let us choose a random vector x . Expanding it the singular vector basis v_i of B , we get $x = c_i v_i$. Let σ_i be the corresponding eigenvalue of v_i . Applying B 'k' times to the above equation and taking dot product with v_1 , we can see that after some iterations, the x vector will shift to v_1 since the coefficient corresponding to the first singular vector dominates all of the others. And so if we normalize, the coefficient of $B^k x$ corresponding to v_1 tends to 1, while the rest tend to zero. We won’t compute a precise number of iterations. Instead we’ll just compute until the angle between $B^{k+1}x$ and $B^k x$ is very small (in the order of ϵ). i.e. we start with a random unit vector x , and then loop computing $x_{s+1} = Bx_s$, re-normalizing at each step. The condition to stop is that the magnitude of the dot product between x_s and x_{s+1} is very close to 1.

We started with the matrix A and computed v_1 . We can use v_1 to compute u_1 and $\sigma_1(A)$. Now, let us ignore all vectors in the span of v_1 for our next step, and to do this we can simply subtract the rank 1 component of A corresponding to v_1 . i.e., set $A' = A - \sigma_1(A)u_1v_1^T$. Then, we see that $\sigma_1(A') = \sigma_2(A)$ and basically all the singular vectors shift indices by 1 when going from A to A' . Then we can repeat this recursively to get U , V and diagonal elements of Σ . While doing this computation, we assume that $m > n$ by taking n columns as variables and m rows as values for a set of measurement.

References

- [1] http://www.cs.yale.edu/homes/el327/datamining2013aFiles/07_singular_value_decomposition.pdf
- [2] <https://gregorygundersen.com/blog/2018/12/20/svd-proof/#:~:text=The%20existence%20claim%20for%20the,existence%20proof%20for%20the%20SVD>

[3] <https://www.itl.nist.gov/div898/handbook/pmc/section5/pmc541.htm>

[4] https://ergodic.ugr.es/cphys/LECCIONES/FORTRAN/power_method.pdf

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