Singular value decomposition (SVD)

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This section will discuss singular value decomposition (SVD) of a matrix $A \in \mathbb{R}^{m \times n}$.

1 Construction

1 1

The first singular value is defined as:

$$\sigma_1 = \sup_{\|v\|=1} \|Av\|.$$

Remark 1. The first singular value is well defined, i.e., such a $v_1 \in \mathbb{R}^n$ always exists. Non-rigorous argument: the function : $v \to ||Av||$ is continuous and with a compact domain.

Now one can find $u_1 \in \mathbb{R}^m$ with $||u_1|| = 1$ such that $Av_1 = \sigma_1 u_1$.

One can follow the definition of the first singular value and define the second singular value as,

$$\sigma_2 = \sup_{\|v\| = 1, v \perp v_1} \|Av\|.$$

The remark $\boxed{1}$ implies that such a v_2 always exists and let us denote it as v_2 . In addition, we can find $u_2 \in \mathbb{R}^m$ with $||u_2|| = 1$ such that $Av_2 = \sigma_2 u_2$.

Remark 2. $\sigma_2 \leq \sigma_1$ because v_2 is taken from a smaller subspace $\{v_1\}^{\perp} \subset \mathbb{R}^n$.

Theorem 1.1. u_1 and u_2 which are defined above are orthogonal.

The theorem implies that $u_1 \perp u_2$. Repeat the process, one can find a unit vector $v_3 \in W_2 = \{v_1, v_2\}^{\perp}$ such that it admits

$$\sigma_3 = \sup_{\|v\|=1, v \in V_2} \|Av\|.$$

In addition, one can find a unit vector u_3 such that $Av_3 = \sigma_3 u_3$. One can show that $\{u_1, u_2, u_3\}$ are orthogonal.

Remark 3. Let us define $W_p = \{v_1, v_2, ..., v_p\}^{\perp}$. If $\sup_{v \in W_p} ||Av|| = 0$, or, $Av_{p+1} = 0$, we can make u_{p+1} (nonzero if possible) to be any vector which is orthogonal to $\{u_1, ..., u_p\}$. If u_{p+1} has to be zero, $span\{u_1, ..., u_p\} = \mathbb{R}^m$

Repeat the process for n times (why is n the maximum step of the process?), we then can construct an orthonormal matrix $V = [v_1, ..., v_n] \in \mathbb{R}^{n \times n}$, another matrix with orthonormal columns $U = [u_1, ..., u_n] \in \mathbb{R}^{m \times n}$ up to some 0 columns, and a diagonal matrix $\Sigma \in \mathbb{R}^{n \times n}$ with diagonal entries being $\sigma_1, ..., \sigma_n$ (up to some 0). Recall the matrix multiplication we have,

$$AV = U\Sigma$$
.

$$|| F_{1} \wedge A \vee_{1} || = 1, \\ || A \vee_{1} || = 6, || A \vee_{1} || = 6, || A \vee_{1} || = 1.$$

$$|| A \vee_{1} || = \frac{|| A \vee_{1} ||}{|| G_{1}} = \frac{|| A \vee_{1} ||}{|| G_{1}} = 1.$$

Orthogonal
Thm I.I.

Remark.

u, uz uz are
orthogonal
Thm 1.1.

3. Q: suppose
$$V_p = span \{V_1 - V_p\}$$

with $S_1 - S_p \neq 0$ | but.

 $S_p \neq 1 = S_p \neq 1$ | $S_p \neq 1$ | $S_$

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$$N_3 = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$
 (pointinct V_3)

$$\overline{S}: \qquad \overline{Q}: \qquad \overline{M}_{2} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \qquad \overline{M}_{2} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \qquad \overline{G}_{3} = 0$$

$$\overline{M}_{3} = 0$$

$$\begin{cases} A V_{1} = 6_{1} V_{1} \\ A V_{2} = 6_{2} V_{2} \\ -\frac{1}{2} & \frac{1}{2} & \frac{1$$

Denote
$$V = [V_1 V_2 - V_n] \in \mathbb{R}^n$$
, V is orthogonal matrix

$$\sum = \left(\begin{array}{c} Q & Q \\ Q & \end{array} \right) \in \mathbb{K}.$$

Full SVD. A
$$\in \mathbb{R}^{n \times n}$$
, $m > n$

$$A = \bigcup Z \bigcup^{\dagger}$$

$$W_{1} = \bigcup_{R} W_{1} = \bigcup_{R} W_{2} = \bigcup_{R} W_{1} = \bigcup_{R} W_{2} = \bigcup_{R} W_{2} = \bigcup_{R} W_{1} = \bigcup_{R} W_{2} = \bigcup_{R} W$$

OF 12 also unitary.

$$Fall SVD \rightarrow A = \begin{bmatrix} U & U_{n+1} & U_{m} \\ U & U_{n+1} & U_{m} \\ U & U_{m} & U_{m} \\ U & U_{m} & U_{m} \\ U & U_{m} & U_{m} \\ U_{m} & U_{m} & U_{m} \\ U_{$$

Theorem 1.2. rank(A) equals to the number of nonzero singular values.

Proof. Let us assume $\{\sigma_1, ..., \sigma_p\}$ are all nonzero singular values but $\sigma_{p+1} = 0$. Let $V_p = \{v_1, ..., v_p\}$ be the singular vector corresponding to $\sigma_1, ... \sigma_p$. We claim that $V_p \subset row(A)$. We have $AV = U\Sigma$, or $U^TA = \Sigma V^T$. The i-th row $(i \leq p)$ of the right-hand side is $\sigma_i v_i^t$. The i-th row on the left-hand side is $(u_i)^t A$, it follows that $v_i^t = \frac{1}{\sigma_i}(u_i)^t A$. This implies that $V_p \subset row(A)$.

By theorem in the last section (Complement theorem), $null(A) = row(A)^{\perp} \subset V_p^{\perp}$. Now, for $v \in V_p^{\perp}$, we have Av = 0, otherwise contradicts with the definition of V_p . As a result, $V_p^{\perp} \subset null(A)$, i.e., $V_p^{\perp} = null(A)$. By the rank theorem, $dim(V_p) = rank(A)$.

As a corollary, $V_p = row(A)$. We summarize the results in the following theorem.

Theorem 1.3. Assume $\{\sigma_1, ..., \sigma_p\}$ are all nonzero singular values, $\{v_1, ..., v_p\}$ and $\{u_1, ..., u_p\}$ are right and left singular vectors respectively, we denote the space spanned by them as V_p and U_p . The followings are true:

$$V_p = row(A),$$

 $U_p = col(A).$

Proof. The first one is proved in the last theorem and let us prove $U_p = col(A)$. We claim that for any $y \in \mathbb{R}^n$, there exists $x \in row(A)$ such that Ax = Ay. When $y \in row(A)$, it is true. When $y \notin row(A)$, assume not, i.e., for all $x \in row(A)$, A(x - y) = 0. This implies that $x - y \in row(A)$. It follows from the theorem we discussed in the last section that $x - y \in row(A)$. However, this is the contradiction. The claim is proved.

Now for any $y \in \mathbb{R}^n$, let $y_x \in row(A)$ such that $Ay_x = Ay$. Since $V_p = row(A)$, $y_x = \sum_{i=1}^p c_i^y v_i$ for some constants c_i . It follows that $Ay = \sum_i \sigma_i c_i^y u_i$. The other direction is also true, this implies that $col(A) = U_p$.

Full SVD: make U matrix orthonormal when m > n. One can append an additional m - n orthonormal columns to fulfill this goal. Σ should change as well so that the product $AV = U\Sigma$ still holds. To do this, one can append m - n zero rows to the bottom of Σ . As a result, we have $AV = U\Sigma$ where $V \in \mathbb{R}^{n \times n}$, $U \in \mathbb{R}^{m \times m}$ and $\Sigma \in \mathbb{R}^{m \times n}$. Since V is orthonormal, we have:

$$A = U\Sigma V^{-1}$$

2 Revisit SVD

2.1 From SVD

Let $A \in \mathbb{R}^{m \times n}$. Suppose A admits an SVD $A = U\Sigma V^t$, where $U \in \mathbb{R}^{m \times m}$, $V \in \mathbb{R}^{n \times n}$ are orthogonal matrices and $\Sigma \in \mathbb{R}^{m \times n}$ is a diagonal matrix. Let us know consider $AA^t \in \mathbb{R}^{m \times n}$ and $A^tA \in \mathbb{R}^{n \times n}$, which are symmetric matrices.

$$\begin{split} A^t A &= V \Sigma^t U^t U \Sigma V^t = V \Sigma^t \Sigma V^t, \\ A A^t &= U \Sigma V^t V \Sigma^t U^t = U \Sigma \Sigma^t U^t. \end{split}$$

 $\Sigma\Sigma^2$ and $\Sigma^2\Sigma$ are still diagonal, and nonzero entries of these two matrices are indeed singular values squared.

In addition, since U and V are orthogonal (hence invertible), this implies that $V\Sigma^t\Sigma V^t$ and $U\Sigma \Sigma^t U^t$ are the eigenvalue decomposition (diagonalization) of A^tA and AA^t (theorem 4.1 in diagonalization section).

2.2 From eigenvalue decomposition

 A^tA is symmetric and by the Spectral theorem, let $\{v_i\}_{i=1}^n$ be the orthonormal eigenvectors of A^tA corresponding to eigenvalue $\lambda_1 \geq \lambda_2 ... \geq \lambda_n$. We first claim that $\lambda_1 \geq \lambda_2 ... \geq \lambda_n \geq 0$. We have,

$$||Av_i||^2 = (Av_i)^t Av_i = v_i^t A^t Av_i = \lambda_i ||v||^2 \ge 0,$$

it implies that $\lambda_i \geq 0$.

Let $\sigma_1 = \sqrt{\lambda_1}$ for all i. We want to find $\{u_k\}_k$, which are orthonormal, such that,

$$Av_k = \sigma_k u_k.$$

When $\sigma_k \neq 0$, one can define $u_k = \frac{1}{\sigma_k} A v_k$. Let us claim all u_k are orthonormal. Let u_i, u_j be nonzero and defined as before. We have,

$$u_i^t u_j = \frac{1}{\sigma_i \sigma_j} v_i^t A^t A v_j = v_i^t v_j = \delta_{ij}.$$

The claim is proved. When $\lambda_p = 0$, for some $1 \leq p \leq n$, we can construct u_p which is orthogonal to $u_1, u_2, ..., u_{p-1}$. If $\{u_1, ..., u_{p-1}\}$ have formed a basis for \mathbb{R}^m , then set $u_p = 0$. Now we can construct an orthonormal matrix $V = [v_1, ..., v_n] \in \mathbb{R}^{n \times n}$, another matrix with orthonormal columns $U = [u_1, ..., u_n] \in \mathbb{R}^{m \times n}$ up to some 0 columns, and a diagonal matrix $\Sigma \in \mathbb{R}^{n \times n}$ with diagonal entries being $\sigma_1, ..., \sigma_n$. The SVD follows: $AV = U\Sigma$. One can apply the same trick as before to make U a square matrix and obtain the full SVD.

Remark 4. Nonzero u_k constructed before are eigenvectors of AA^t . The proof is simple.

$$AA^tu_k = AA^t\frac{1}{\sigma_k}Av_k = A\frac{1}{\sigma_k}A^tAv_k = A\sigma_kv_k = \sigma_k^2u_k.$$

Remark 5. If $S = S^t$ is symmetric and assumes all eigenvalues are non-negative, then the eigenvalue decomposition is the SVD (as long as the eigenvalues are in descending order).

3 Rank k approximation

Let us consider the SVD of $A \in \mathbb{R}^{m \times n}$, i.e., $A = U\Sigma V^t$. Recall the matrix multiplication, we have a decomposition for A as,

$$A = \sum_{i=1}^{n} \sigma_i u_i v_i^t = \sum_{i=1}^{r} \sigma_i u_i v_i^t,$$

where $\{\sigma_i\}_{i=1}^r$ are all nonzero singular values of A. Let us define an approximation A_k to A as:

$$A_k = \sum_{i=1}^k \sigma_i u_i v_i^t,$$

where $k \leq r$. It is easy to check $rank(A_k) = k$. We then can show A_k is the best approximation to A; the result is summarized in the following theorem.

3.1 Preliminaries

Definition 3.1. L^2 norm of a matrix $A \in \mathbb{R}^{m \times n}$ is defined as:

$$||A||_2 = \max_{x \in \mathbb{R}^n, ||x|| = 1} ||Ax|| = \max_{x \in \mathbb{R}^n, x \neq 0} \frac{||Ax||}{||x||} = \sigma_1.$$

In the rest of the notes, we sometimes write $\|\cdot\|_2$ as $\|\cdot\|$ for simplicity.

Remark 6. For any $x \in \mathbb{R}^n$ and $x \neq 0$, we have, $\frac{\|Ax\|}{\|x\|} \leq \|A\|_2$. This implies that $\|Ax\| \leq \|A\| \|x\|$.

3.2 Eckart-Young theorem

Theorem 3.2 (Eckart-Young). Suppose $A, B \in \mathbb{R}^{m \times n}$ and $rank(B) = k \leq rank(A) = r$. We then have:

$$||A - B|| \ge ||A - A_k|| = \sigma_{k+1}.$$

That is A_k is the best $rank \ k$ approximation to A in the L^2 sense.

Proof. We first prove that $||A - A_k|| = \sigma_{k+1}$. We have,

$$A - A_k = \sum_{i=k+1}^{n} \sigma_i u_i v_i^t = \sum_{i=1}^{n-k} \sigma_{i+k} u_{i+k} v_{i+k}^t + \sum_{i=n-k+1}^{n} \tilde{\sigma}_i \tilde{u}_i \tilde{v}_i^t,$$

where $\tilde{\sigma}_i = 0$, \tilde{u}_i are orthonormal to all u_{i+k} , and \tilde{v}_i are also orthonormal to all v_{i+k} . The summation is then an SVD of $A - A_k$. Since $||A - A_k||$ is equal to the first singular value of its SVD, we have $||A - A_k|| = \sigma_{k+1}$.

Assume not, i.e., assume there is $B \in \mathbb{R}^{m \times n}$ with rank(B) = k such that $||A - B|| < ||A - A_k|| = \sigma_{k+1}$. For any $w \in \mathbb{R}^n$, we have $||(A - B)w|| < \sigma_{k+1}||w||$. It follows that, for any $w \in null(B)$, we have,

$$||(A - B)w|| = ||Aw|| < \sigma_{k+1}||w||. \tag{1}$$

Now for any $w \in V_{k+1} = span\{v_1, v_2, ..., v_{k+1}\}$, we claim that $||Aw|| \ge \sigma_{k+1}||w||$. Since $w \in V_{k+1}$, there exist $c_1, ..., c_{k+1}$, such that $w = \sum_{i=1}^{k+1} c_i v_i$. It follows that

$$||Aw|| = ||\sum_{i=1}^{k+1} c_i A v_i|| = \sum_{i=1}^{k+1} |c_i| \sigma_i \ge \sigma_{k+1} ||w||,$$
(2)

where the last inequality is due to the orthogonality of v_i and $\sigma_1 \geq ... \geq \sigma_{k+1}$.

The Rank theorem indicates that dim(null(B)) = n - k, however $dim(V_{k+1}) = k + 1$. We then have $dim(null(B)) + dim(V_{k+1}) > n$. Since null(B) and V_{k+1} both are subspace of \mathbb{R}^n , this implies that there exists $w \neq 0$ such that $w \in null(B) \cap V_{k+1}$. However, $\boxed{1}$ and $\boxed{2}$ cannot hold simultaneously, which is the contradiction.

Corollary 3.2.1. Suppose $A, B \in \mathbb{R}^{m \times n}$ and $rank(B) \le k \le rank(A) = r$. We then have:

$$||A - B|| \ge ||A - A_k|| = \sigma_{k+1}.$$

Proof. Let rank(B) = k - j, $0 \le j \le k$, by Eckart-Young, we have $||A - B|| \ge ||A - A_{k-j}|| = \sigma_{k-j+1} \ge \sigma_{k+1} = ||A - A_k||$.

3.3 Eckart-Young theorem (Frobenius)

Definition 3.3. The Frobenius norm of $A \in \mathbb{R}^{m \times n}$ is:

$$||A||_F = \sqrt{\sum_{i=1}^m \sum_{j=1}^n a_{ij}^2}.$$

Theorem 3.4. Frobenius norm can be calculated in the following way,

$$||A||_F^2 = \sum_i \sigma_i^2.$$

Corollary 3.4.1. Let the SVD of A be $A = U\Sigma V^t$, and $U = [u_1, ..., u_n], V = [v_1, ..., v_n]$, and the diagonal entries of Σ are $\sigma_1, ..., \sigma_n$. Let $A_k = \sum_{i=1}^k \sigma_i u_i v_i^t$, we have,

$$||A - A_k||_F^2 = \sum_{i=k+1}^n \sigma_i^2.$$

Theorem 3.5 (Courant Fisher min max). For $A \in \mathbb{R}^{m \times n}$, the singular value σ_i of A satisfy:

$$\sigma_{k} = \max_{V \subset \mathbb{R}^{n}, dim(V) = k} \min_{v \in V, ||v|| = 1} ||Av||,$$

$$\sigma_{k+1} = \min_{V \subset \mathbb{R}^{n}, dimV = n - k} \max_{v \in v, ||v|| = 1} ||Av||.$$

Proof. Let us prove the first one first. Let V be any k- dimensional space. Since $dim(span\{v_k,...,v_n\})=n-k+1$, V intersects $span\{v_k,...,v_n\}$ nontrivially. Let v be a unit vector in the intersection, i.e., there exist $c_k,...,c_n$ such that, $v=\sum_{i=k}^n c_i v_i$. Moreover, $\|v\|=\sum_{i=k}^n |c_i|=1$. We have, $Av=\sum_{i=k}^n c_i\sigma_iu_i$, it follows that, $\|Av\|=\sum_{i=k}^n |c_i|\sigma_i\|u_i\|\leq \sigma_k$. This implies that for any V of dimension k, there exists v such that $\|Av\|\leq \sigma_k$, i.e., $\min_{v\in V,\|v\|=1}\|Av\|\leq \sigma_k$. Now we need to find a V such that the equality sign holds, i.e., $\|Av\|=\sigma_k$. We claim that V can be $span\{v_1,...,v_k\}$, i.e., $V\cap span\{v_k,...,v_n\}=span\{v_k\}$. Now let $v=v_k$, it follows that $\|Av\|=\sigma_k$. The claim is proved, i.e., maximizing over all V, we can obtain the equal sign.

The second one can be derived similarly. Let V be any (n-k)- dimensional subspace of \mathbb{R}^n , it intersects $V_{k+1} := span\{v_1,...,v_{k+1}\}$ nontrivially, i.e., there exists unit vector v in the intersection. It follows that, there exist $c_1,...,c_{k+1}$ such that $v = \sum_{i=1}^{k+1} c_i v_i$. We have $Av = \sum_{i=1}^{k+1} c_i \sigma_i u_i$, it follows that, $||Av|| \geq \sigma_{k+1}$. This implies that for any V of dimension n-k, there exists v such that $||Av|| \geq \sigma_{k+1}$, i.e., $\max_{v \in V, ||v|| = 1} ||Av|| \geq \sigma_{k+1}$. The equality holds when $V = span\{v_{k+1},...,v_n\}$ and $v = v_{k+1}$.

Theorem 3.6 (Weyl). Let $A, B \in \mathbb{R}^{m \times n}$, and denote the singular values as $\sigma_i(A)$ and $\sigma_i(B)$. We then have:

$$\sigma_{i+j-1}(A+B) \le \sigma_i(A) + \sigma_j(B). \tag{3}$$

Proof. Let V_A , and V_B be the subspace of \mathbb{R}^n of dimensions n-k and n-l, which are orthogonal to the first k and l right singular vectors of A and B respectively. Let $W = V_A \cap V_B$, we have $dim(W) \geq n-k-l$. It follows that,

$$\max_{v \in W, ||v|| = 1} ||Av + Bv|| = \max_{v \in W, ||v|| = 1} ||Av|| + ||Bv|| \le \sigma_{k+1} + \sigma_{l+1}.$$

By Curant-Fisher,

$$\sigma_{k+l+1}(A+B) = \min_{V \subset \mathbb{R}^n, dimV = n-k-l} \max_{v \in v, ||v|| = 1} ||Av + Bv|| \le \max_{v \in W, ||v|| = 1} ||Av + Bv|| = \sigma_{k+1} + \sigma_{l+1}.$$

Weyl's inequality will help us prove the Eckart-Young for the Frobenius norm.

Theorem 3.7 (Eckart-Young Frobenius). Suppose $A, B \in \mathbb{R}^{m \times n}$ and $rank(B) = k \leq rank(A) = r$. We then have:

$$||A - B||_F^2 \ge ||A - A_k||_F^2 = \sum_{i=k+1} \sigma_i^2.$$

That is A_k is the best $rank \ k$ approximation to A in the L^2 sense.

Proof. Let X = A - B and Y = B and apply Weyl's inequality 3.6

$$\sigma_{i+k}(A) \le \sigma_i(A-B) + \sigma_{k+1}(B) = \sigma_i(A-B),$$

where is last equal sign is due to rank(B) = k. Apply Corollary 3.4.1 it follows that,

$$||A - A_k||_F^2$$

$$= \sum_{i=k+1}^{r} \sigma_i(A)^2 = \sum_{i=1}^{r-k} \sigma_{i+k}^2(A) \le \sum_{i=1}^{r-k} \sigma_i^2(A-B) \le \sum_{i=1}^{\min(m,n)} \sigma_i^2(A-B) = ||A-B||_F^2.$$

A direct consequence of the Eckart-Young for the Frobenius norm is the proper orthogonal decomposition (POD).

3.4 Proper orthogonal decomposition (POD)

Given $A = [y_1, y_2, ..., y_n] \in \mathbb{R}^{m \times n}$, and a set of orthonormal vectors $Q = [x_1, ..., x_k] \in \mathbb{R}^{m \times k}$, one wants to solve the following problem:

$$\min_{Q} \sum_{i=1}^{n} \|y_i - \sum_{j=1}^{k} \langle y_i, x_j \rangle x_j \|^2.$$
(4)

We claim that the equation 4 is equivalent to the matrix form,

$$\sum_{i=1}^{n} \|y_i - \sum_{j=1}^{k} \langle y_i, x_j \rangle x_j \|^2 = \|A - QQ^t A\|_F.$$
 (5)

Denote the matrix as columns, i.e., $||A - QQ^tA||_F = ||[y_1 - QQ^Ty_1, ..., y_n - QQ^ty_n]||_F$; and denote $y_i - QQ^Ty_i$ as $z_i \in \mathbb{R}^m$, it follows that,

$$||[y_1 - QQ^T y_1, ..., y_n - QQ^t y_n]||_F^2 = \sum_{i=1}^n \sum_{j=1}^m z_{ji}^2 = \sum_{i=1}^n ||z_i||^2 = \sum_{i=1}^n ||y_i - QQ^t y_i||^2.$$

It is not hard to see $QQ^ty_i = \sum_{j=1}^k \langle y_i, x_j \rangle x_j$. The claim is proved. Apply the Eckart-Young theorem for the Frobenius norm; we then have the POD theorem.

Theorem 3.8. Given $A = [y_1, y_2, ..., y_n] \in \mathbb{R}^{m \times n}$ with rank r. For any $k \leq r$, we consider,

$$\min_{Q} \sum_{i=1}^{n} \|y_i - \sum_{j=1}^{k} \langle y_i, x_j \rangle \|x_j\|^2,$$
(6)

where $Q = [x_1, ..., x_k] \in \mathbb{R}^{m \times k}$ is a set of orthonormal vectors. The minimum is given by the left singular vectors of A, which are also called proper orthogonal modes. Denote the singular values of A as σ_i , the minimum is equal to $\sum_{i=k+1}^r \sigma_i^2$.

Proof. The only statement left to prove is $QQ^TA = A_k$ if $Q = [u_1, ..., u_k]$ and u_k are the singular vectors. We have,

$$QQ^{T}A = [u_1, u_2, ..., u_k][u_1, u_2, ..., u_k]^{t}A = \sum_{i=1}^{k} u_i u_i^{t}A.$$