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

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 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. $\sigma_2 \le \sigma_1$ 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,

$$AV = U\Sigma.$$

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 $U^T A = \Sigma V^T$. The $i-th$ row ($i \le p$) 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, $V_p^\perp \subset null(A) = row(A)^\perp$, or, $row(A) \subset V_p$. It follows that $V_p = row(A)$. We then have $dim(V_p) = rank(A)$. □

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:

$$
\begin{aligned}
V_p &= row(A), \\
U_p &= col(A).
\end{aligned}
$$

Proof. The first one is proved in the last theorem and let us prove $U_p = col(A)$. Since V is unitary, for any $y \in \mathbb{R}^n$, there exists c_i, $u = 1, ..., n$ such that $y = \sum_{i=1}^n c_i v_i$. It follows that $Ay = \sum_{i=1}^n c_i A v_i = \sum_{i=1}^p c_i \sigma_i u_i$. This implies that $col(A) \subset span\{u_1, ..., u_p\}$. However, $u_i = \frac{1}{\sigma_i} A v_i$, this implies that $u_i \in col(A)$.

□

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 $U \in \mathbb{R}^{m\times n}$ (U is orthogonal if this is the full SVD), $V \in \mathbb{R}^{n\times n}$ are orthogonal matrices and $\Sigma \in \mathbb{R}^{m\times n}$ is a diagonal matrix. Let us now consider $AA^t \in^{m\times m}$ and $A^t A \in \mathbb{R}^{n\times n}$, which are symmetric matrices.

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

$\Sigma\Sigma^2$ 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 (U is orthogonal only when the SVD is full), this implies that $V\Sigma^t\Sigma V^t$ and $U\Sigma\Sigma^t U^t$ are the eigenvalue decomposition (diagonalization) of $A^t A$ and AA^t.

2.2 From eigenvalue decompostion

Let us recall the Spectral theorem.

Theorem 2.1 (Spectral Theorem)**.** Let $A \in \mathbb{C}^{n\times n}$. Then A is Hermitian if and only if there is a unitary matrix $U \in \mathbb{C}^{n\times n}$ and a real diagonal matrix $D \in \mathbb{R}^{n\times n}$ such that $A = UDU^*$.

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,

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

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 $u_k = \frac{1}{\sigma_k} Av_k$. 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.

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

Definition 2.2. 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 5. For any $x \in \mathbb{R}^n$ and $x \neq 0$, we have, $\frac{\|Ax\|}{\|x\|} \leq \|A\|_2$. This implies that $\|Ax\| \leq \|A\|\|x\|$.

Definition 2.3. 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 2.4. Frobenius norm can be calculated in the following way,

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

Proof. Let the SVD be $A = U\Sigma V^t$. We have $\|A\|_F^2 = trace(A^tA)$, it follows that,

$$\|A\|_F^2 = trace(V\Sigma^tU^tU\Sigma V^t) = trace(V\Sigma^t\Sigma V^t) = trace(\Sigma\Sigma^t) = \sum_i \sigma_i^2,$$

where we use $trace(MN) = trace(NM)$ in the last equality, where M and N are two matrices of the proper size. □

Theorem 2.5 (Courant Fisher min max)**.** For $A \in \mathbb{R}^{m\times n}$, the singular value σ_i of A satisfy:

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

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, $v = \sum_{i=k}^n c_iv_i$. Moreover, $\|v\| = \sum_{i=k}^n |c_i| = 1$. We have, $Av = \sum_{i=k}^n c_i\sigma_iu_i$, it follows that, $\|Av\| = \sum_{i=k}^n |c_i|\sigma_i\|u_i\| \le \sigma_k$. This implies that for any V of dimension k, there exists v such that $\|Av\| \le \sigma_k$, i.e., $\min_{v\in V, \|v\|=1} \|Av\| \le \sigma_k$. 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 $v = \sum_{i=1}^{k+1} c_iv_i$. We have $Av = \sum_{i=1}^{k+1} c_i\sigma_iu_i$, it follows that, $\|Av\| \ge \sigma_{k+1}$. This implies that for any V of dimension $n-k$, there exists v such that $\|Av\| \ge \sigma_{k+1}$, i.e., $\max_{v\in V, \|v\|=1} \|Av\| \ge \sigma_{k+1}$. The equality holds when $V = span\{v_{k+1}, ..., v_n\}$ and $v = v_{k+1}$. □

Theorem 2.6. Every matrix A has an SVD. Furthermore, the singular values are unique. If A is square and all σ_i are distinct, the left and right singular vectors are unique up to complex scalar signs (complex scalar factors of absolute value 1).

Remark 6. If $A = U\Sigma V^t$, where U has orthonormal columns, V is orthogonal, and Σ is diagonal and has non-negative diagonal entries, then this is an SVD of A.

Proof. $A^TA = V\Sigma^t\Sigma V^T$, it is then very easy to see the column of V are the eigenvectors of A^TA, or they are singular vectors of A. Similarly, $\Sigma^t\Sigma$ diagonal entries are eigenvalues of A^TA, and their positve square roots are singular values of A. □

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,

$$A = \sum_{i=1}^n \sigma_iu_iv_i^t = \sum_{i=1}^r \sigma_iu_iv_i^t,$$

→ # non-zero singular values.

Remark 6.

$$A = U \Sigma V^t \qquad \Sigma = \begin{pmatrix} \sigma_1 & & \\ & \ddots & \\ & & \sigma_n \end{pmatrix} \qquad \Sigma^t \Sigma = \begin{pmatrix} \sigma_1^2 = \lambda_1 & & \\ & \ddots & \\ & & \sigma_n^2 = \lambda_n \end{pmatrix}$$

$$A^t A = V \Sigma^t \underbrace{U^t U}_{I} \Sigma V^t = V \Sigma^t \Sigma V^t$$

$\Rightarrow$ $V \underbrace{(\Sigma \Sigma^t)}_{D} V^t$ is an eigenvalue decomposition of $A^t A$.

$\Rightarrow$ e.vals of $A^t A$ is the square of the singular values of A.

Because the singular values of A $:= \sqrt{\text{e.val of } A^t A}$

$\Rightarrow$ Σ stores all singular values of A.

Sec 3.

Want to find a reduced order model (ROM) ("simplified") to approximate the full model

The process of obtaining the ROM is called model reduction.

① extract the most important features

② remove irrelevant informations.

$A \in \mathbb{R}^{m \times n}$, want to find a matrix B_k of rank k,

B_k can approximate A in some sense.

$\text{rank}(B_k) \ll \text{rank}(A)$

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

Definition

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

$$\text{rank}(A_k) = k$$

pf

$$A_k = \sum_{i=1}^{k} \sigma_i u_i v_i^t + \sum_{i=k+1}^{n} \tilde{\sigma}_i \tilde{u}_i \tilde{v}_i^t$$

$\sigma_i > 0$

$\tilde{\sigma}_i = 0$

$\tilde{u}_i$, all $\tilde{u}_i$ are orthonormal to u_i $(i = 1, \ldots, k)$

$\tilde{v}_i$, all $\tilde{v}_i$ are orthogonal to v_i $(i = 1, \ldots, k)$

$$A_k = \tilde{U} \tilde{\Sigma} \tilde{V}^t$$

$\tilde{U} = [u_1, \ldots u_k, \tilde{u}_{k+1}, \ldots \tilde{u}_n]$ $\quad \tilde{V} = [v_1, \ldots v_k, \tilde{v}_{k+1}, \ldots \tilde{v}_n]$

$$\tilde{\Sigma} = \begin{pmatrix} \sigma_1 & & & & \\ & \ddots & & & \\ & & \sigma_k & & \\ & & & 0 & \\ & & & & \ddots \\ & & & & & 0 \end{pmatrix}$$

$\Rightarrow$ $\tilde{U} \tilde{\Sigma} \tilde{V}^t$ is an SVD of A_k

$\text{rank}(A_k)$ = # non-zero singular values

$= k$.

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 Eckart-Young theorem

Theorem 3.1 (Eckart-Young)**.** Suppose $A, B \in \mathbb{R}^{m \times n}$ and $rank(B) = k \leq rank(A) = r$. We then have:

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

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 $\|Aw\| \geq \sigma_{k+1}\|w\|$. 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

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

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, 1 and 2 cannot hold simultaneously, which is the contradiction.

□

Corollary 3.1.1. Suppose $A, B \in \mathbb{R}^{m \times n}$ and $rank(B) \leq k \leq rank(A) = r$. We then have:

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

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

3.2 Eckart-Young theorem (Frobenius)

Corollary 3.1.2. 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 3.2 (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:

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

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,

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

By Curant-Fisher,

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

□

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

Theorem 3.3 (Eckart-Young Frobenius)**.** Suppose $A, B \in \mathbb{R}^{m\times n}$ and $rank(B) = k \leq rank(A) = r$. We then have:

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

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 3.2,

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

where is last equal sign is due to $rank(B) = k$. Apply Corollary 3.1.2, it follows that,

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

□

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

3.3 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:

$$\min_Q \sum_{i=1}^{n} \|y_i - \sum_{j=1}^{k} < y_i, x_j > x_j\|^2. \tag{4}$$

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

$$\sum_{i=1}^{n} \|y_i - \sum_{j=1}^{k} < y_i, x_j > x_j\|^2 = \|A - QQ^t A\|_F. \tag{5}$$

Denote the matrix as columns, i.e., $\|A - QQ^t A\|_F = \|[y_1 - QQ^T y_1, ..., y_n - QQ^t y_n]\|_F$; and denote $y_i - QQ^T y_i$ 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 $QQ^t y_i = \sum_{j=1}^{k} < y_i, x_j > x_j$. The claim is proved. Apply the Eckart-Young theorem for the Frobenius norm; we then have the POD theorem.

Theorem 3.4. Given $A = [y_1, y_2, ..., y_n] \in \mathbb{R}^{m\times n}$ with rank r. For any $k \leq r$, we consider,

$$\min_Q \sum_{i=1}^{n} \|y_i - \sum_{j=1}^{k} < y_i, x_j > x_j\|^2, \tag{6}$$

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 $QQ^T A = A_k$ if $Q = [u_1, ..., u_k]$ and u_k are the singular vectors. We have,

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

□