0368-3248-01-Algorithms in Data Mining **Fall 2011**

Lecture 8: Singular Value Decomposition

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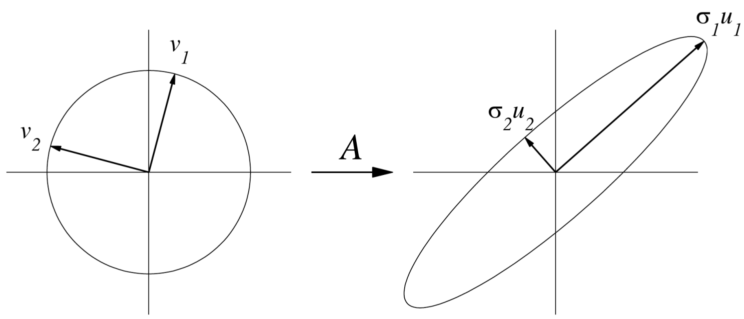
Warning: *This note may contain typos and other inaccuracies which are usually discussed during class. Please do not cite this note as a reliable source. If you find mistakes, please inform me.*

We will see that any matrix $A \in \mathbb{R}^{m\times n}$ can be written as $A = U\Sigma V^T$ such that $U \in \mathbb{R}^{m\times m}$ is unitary, $V \in \mathbb{R}^{n\times n}$ is unitary, and $\Sigma \in \mathbb{R}^{m\times n}$ is a non-negative real diagonal matrix. $\Sigma(i,i)$, denoted σ_i, are unique. If A the singular values are distinct, then the singular vectors are unique up to a multiplication by $z \in \mathbb{C}$ with $|z| = 1$.

Remark 0.1. *Note the difference in notation from what we saw in class. The matrices V and U are what we denoted by $[V;\overline{V}]$ and $[U;\overline{U}]$ respectively. This makes the proofs a little cleaner and hopefully more easy to follow. Note also that Σ , unlike the matrix we denoted by S, is not square. The non square matrix Σ is still diagonal though, i.e. $\Sigma(i,j) = 0$ for all $i \neq j$.*

1 The geometry of SVD



2 Proof of existence

Set $\sigma_1 = \|A\|_2$. Let $u_1 \in \mathbb{R}^n$ and $v_1 \in \mathbb{R}^m$ be unit 2-norm vectors such that $Av_1 = \sigma_1 u_1$. To find these vectors, find the unit vector v_1 that brings to maximum the expression

$$\max_{\|x\|=1} \|Ax\|.$$

Then $Av_1 = \mu u_1$ for some μ and a unit vector u_1. Since $\|Av_1\| = \sigma_1$, we get that $\sigma_1 = \|Av_1\| = |\mu|\,\|u_1\| = |\mu|$. Set $\mu = \sigma_1$ to be positive, by flipping the sign of u_1 if needed.

Complete v_1 into an orthonormal basis of $\mathbb{C}^n$, denote V_1. Complete u_1 into an orthonormal basis of $\mathbb{C}^m$, denoted U_1.

$$S = U_1^T A V_1 = U_1^T\,[\sigma_1 u_1, Av_2, \ldots, Av_n] = \begin{pmatrix} \sigma_1 & w^T \\ 0 & B \end{pmatrix}.$$

We will show that $w^T = 0$.

$$\|S \begin{pmatrix} \sigma_1 \\ w \end{pmatrix}\|_2 = \| \begin{pmatrix} \sigma_1 & w^T \\ 0 & B \end{pmatrix} \begin{pmatrix} \sigma_1 \\ w \end{pmatrix}_2^T \| \geq \sigma_1^2 + w^T w = \sqrt{\sigma_1^2 + w^T w}\| \begin{pmatrix} \sigma_1 \\ w \end{pmatrix}\|_2.$$

That is $\|S\| \geq \sqrt{\sigma_1^2 + w^T w}$. But $\|S\|_2 = \|A\|_2 = \sigma_1$ and so $w = 0$.

By induction, $B = U_2 \Sigma_2 V_2^T$ and

$$A = U_1 S V_1^T = U_1 \begin{pmatrix} 1 & 0 \\ 0 & U_2 \end{pmatrix} \begin{pmatrix} \sigma_1 & 0 \\ 0 & \Sigma_2 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & V_2^T \end{pmatrix} V_1^T.$$

The matrices

$$U = U_1 \begin{pmatrix} 1 & 0 \\ 0 & U_2 \end{pmatrix}, \quad V = V_1 \begin{pmatrix} 1 & 0 \\ 0 & V_2^T \end{pmatrix}$$

are unitary and the proof is complete.

3 More properties of SVD

Lemma 3.1. *The rank of A equals the number of nonzero singular values.*

Proof. Recall that if B is $n \times k$ with rank n than $\text{rank}(AB) = rank(A)$, and if C is $l \times m$ with rank m then $\text{rank}(CA) = rank(A)$. Thus,

$$\text{rank}(A) = \text{rank}(U\Sigma V^T) = \text{rank}(\Sigma V^T) = \text{rank}(\Sigma).$$

Since Σ is diagonal, its rank it the number its nonzero elements. □

Lemma 3.2. *Let* $\text{rank}(A) = r$. *Then,*

$$\begin{aligned} \text{range}(A) &= \text{span}(u_1, \ldots, u_r), \\ \text{null}(A) &= \text{span}(v_{r+1}, \ldots, v_n). \end{aligned}$$

Proof.

$$\begin{aligned} y \in \text{range}(A) &\iff \exists x \text{ such that } y = Ax \\ &\iff y = U\Sigma V^T x \\ &\iff y = U\Sigma z, \text{ where } z = V^T x \\ &\iff y = U\left(\sigma_1 z_1, \ldots, \sigma_r z_r, 0, \ldots, 0\right)^T \\ &\iff y = \sum_{i=1}^{r} (\sigma_i z_i) u_i \\ &\iff y \in \text{span}(u_1, \ldots, u_r). \end{aligned}$$

$$\begin{aligned} x \in \text{null}(A) &\iff \|Ax\|_2 = 0 \iff \|U\Sigma V^T x\|_2 = 0 \\ &\iff \|\Sigma V^T x\|_2 = 0 \iff \|\Sigma y\|_2 = 0 \text{ where } y = V^T x \\ &\iff y = (0, \ldots, 0, y_{r+1}, \ldots, y_n)^T \text{ where } y = V^T x \\ &\iff x = Vy, \; y = (0, \ldots, 0, y_{r+1}, \ldots, y_n)^T \\ &\iff x = \sum_{i=r+1}^{n} y_i v_i \\ &\iff x \in \text{span}(v_{r+1}, \ldots, v_n). \end{aligned}$$

□

Lemma 3.3. $\|A\|_2 = \sigma_1$ *(even if you don't know the above proof).*

Proof. Immediate from the invariance of $\|\cdot\|_2$ under unitary transformations. □

Similarly, $\|A\|_F = (\sigma_1^2 + \cdots + \sigma_r^2)^{1/2}$.

4 Relation between singular values and eigenvalues

Lemma 4.1. *The singular values of A are the square roots of the nonzero eigenvalues of A^TA and AA^T.*

Proof. If $A = U\Sigma V^T$, then $A^T = V\Sigma U^T$ and

$$AA^T = \left(U\Sigma V^T\right)\left(V\Sigma U^T\right) = U\Sigma\Sigma U^T = U\Sigma^2U^{-1}.$$

AA^T is positive semi-definite and therefore all eigenvalues are non-negative and there is no problem with the square root. □

Do not use this observation to compute the SVD! Reason: Assume for simplicity that we have a 2×2 matrix A (not diagonal) whose SVD is given by $A = \sigma_1 u_1 v_1^T + \sigma_2 u_2 v_2^T$ (See 5.1 below). If $\sigma_2/\sigma_1 < 10^{-15}$, then the second term will disappear due to round-off, that is, we cannot represent such a matrix in double precision. Now, if the matrix A has $\sigma_2/\sigma_1 < 10^{-8}$, then A^TA and AA^T have ratio of singular values that is smaller than 10^{-15}, and so those matrices cannot be represented, and will be approximated as rank-1 matrices with the second singular value being due to round-off. In other words, although A is not terribly conditioned, we loose the small eigenvalues if we try to compute the SVD by computing the eigenvalues of A^TA or AA^T.

Lemma 4.2. *If A is hermitian, then the singular values of A are the absolute values of its eigenvalues.*

Proof. A hermitian matrix is diagonalized by a unitary matrix with real eigenvalues. That is,

$$A = Q\Lambda Q^T = Q\,|\Lambda|\,\mathrm{sign}(\Lambda)Q^T.$$

Now set $U = Q$, $\Sigma = |\Lambda|$, $V^T = \mathrm{sign}(\Lambda)Q^T$. □

5 Approximation properties

5.1 Rank-k approximation in the spectral norm

Lemma 5.1. *A can be written as a sum of rank-1 matrices. Explicitly,*

$$A = \sum_{j=1}^{r} \sigma_j u_j v_j^T.$$

Theorem 5.1. *Set*

$$A_k = \sum_{j=1}^{k} \sigma_j u_j v_j^T.$$

Then,

$$\min_{\substack{B\in\mathbb{C}^{m\times n}\\ \mathrm{rank}(B)\le k}} \|A - B\|_2 = \|A - A_k\|_2 = \sigma_{k+1}.$$

Proof.

$$A - A_k = \sum_{j=1}^{r} \sigma_j u_j v_j^T - \sum_{j=1}^{k} \sigma_j u_j v_j^T = \sum_{j=k+1}^{r} \sigma_j u_j v_j^T$$

and thus σ_{k+1} is the largest singular value of $A - A_k$. Alternatively, look at $U^TA_kV = \mathrm{diag}(\sigma_1, \ldots, \sigma_k, 0, \ldots, 0)$, which means that $\mathrm{rank}(A_k) = k$, and that

$$\|A - A_k\|_2 = \|U^T(A - A_k)V\|_2 = \|\,\mathrm{diag}(0, \ldots, 0, \sigma_{k+1}, \ldots, \sigma_r)\|_2 = \sigma_{k+1}.$$

Let B be an arbitrary matrix with $\operatorname{rank}(B_k) = k$. Then, it has a null space of dimension $n-k$, that is,

$$\operatorname{null}(B) = \operatorname{span}(w_1, \ldots, w_{n-k}).$$

A dimension argument shows that

$$\operatorname{span}(w_1, \ldots, w_{n-k}) \cap \operatorname{span}(v_1, \ldots, v_{k+1}) \neq \{0\}.$$

Let w be a unit vector from the intersection. Since

$$Aw = \sum_{j=1}^{k+1} \sigma_j (v_j^T w) u_j,$$

we have

$$\|A - B\|_2^2 \geq \|(A-B)w\|_2^2 = \|Aw\|_2^2 = \sum_{j=1}^{k+1} \sigma_j^2 \left|v_j^T w\right|^2 \geq \sigma_{k+1}^2 \sum_{j=1}^{k+1} \left|v_j^T w\right|^2 = \sigma_{k+1}^2,$$

since $w \in \operatorname{span}\{v_1, \ldots, v_{n+1}\}$, and the v_j are orthogonal. □

5.2 Rank-k approximation in the Frobenius norm

The same theorem holds with the Frobenius norm.

Theorem 5.2. *Set*

$$A_k = \sum_{j=1}^{k} \sigma_j u_j v_j^T.$$

Then,

$$\min_{\substack{B \in \mathbb{C}^{m \times n} \\ \operatorname{rank}(B) \leq k}} \|A - B\|_F = \|A - A_k\|_F = \sqrt{\sum_{i=k+1}^{n} \sigma_i^2}.$$

Proof. Suppose $A = U\Sigma V^T$. Then

$$\min_{\operatorname{rank}(B) \leq k} \|A - B\|_F^2 = \min_{\operatorname{rank}(B) \leq k} \|U\Sigma V^T - UU^T BVV^T\|_F^2 = \min_{\operatorname{rank}(B) \leq k} \|\Sigma - U^T BV\|_F^2.$$

Now,

$$\|\Sigma - U^T BV\|_F^2 = \sum_{i=1}^{n} \left(\Sigma_{ii} - \left(U^T BV\right)_{ii}\right)^2 + \text{off-diagonal terms.}$$

If B is the best approximation matrix and $U^T BV$ is not diagonal, then write $U^T BV = D + O$, where D is diagonal and O contains the off-diagonal elements. Then the matrix $B = UDV^T$ is a better approximation, which is a contradiction.

Thus, $U^T BV$ must be diagonal. Hence,

$$\|\Sigma - D\|_F^2 = \sum_{i=1}^{n} (\sigma_i - d_i)^2 = \sum_{i=1}^{k} (\sigma_i - d_i)^2 + \sum_{i=k+1}^{n} \sigma_i^2,$$

and this is minimal when $d_i = \sigma_i$, $i = 1, \ldots, k$. The best approximating matrix is $A_k = UDV^T$, and the approximation error is $\sqrt{\sum_{i=k+1}^{n} \sigma_i^2}$. □

5.3 Closest orthogonal matrix

The SVD also allows to find the orthogonal matrix that is closest to a given matrix. Again, suppose that $A = U\Sigma V^T$ and W is an orthogonal matrix that minimizes $\|A - W\|_F^2$ among all orthogonal matrices. Now,

$$\|U\Sigma V^T - W\|_F^2 = \|U\Sigma V^T - UU^T W V V^T\| = \|\Sigma - \tilde{W}\|,$$

where $\tilde{W} = U^T W V$ is another orthogonal matrix. We need to find the orthogonal matrix $\tilde{W}$ that is closest to Σ. Alternatively, we need to minimize $\|\tilde{W}^T\Sigma - I\|_F^2$.

If U is orthogonal and D is diagonal and positive, then

$$\begin{aligned} \operatorname{trace}(UD) = \sum_{i,k} u_{ik} d_{ki} &\leq \sum_i \left(\left(\sum_k u_{ik}^2 \right)^{1/2} \left(\sum_k d_{ik}^2 \right)^{1/2} \right) \\ &= \sum_i \left(\sum_k d_{ki}^2 \right)^{1/2} = \sum_i \left(d_{ii}^2 \right)^{1/2} = \sum_i d_{ii} = \operatorname{trace}(D). \end{aligned} \tag{1}$$

Now

$$\begin{aligned} \|\tilde{W}^T\Sigma - I\|_F^2 &= \operatorname{trace}\left(\left(\tilde{W}^T\Sigma - I \right) \left(\tilde{W}^T\Sigma - I \right)^T \right) \\ &= \operatorname{trace}\left(\left(\tilde{W}^T\Sigma - I \right) \left(\Sigma\tilde{W} - I \right) \right) \\ &= \operatorname{trace}\left(\tilde{W}^T\Sigma^2\tilde{W} \right) - \operatorname{trace}\left(\tilde{W}^T\Sigma \right) - \operatorname{trace}\left(\Sigma\tilde{W} \right) + n \\ &= \operatorname{trace}\left(\left(\Sigma\tilde{W} \right)^T \left(\Sigma\tilde{W} \right) \right) - 2\operatorname{trace}\left(\Sigma\tilde{W} \right) + n \\ &= \|\Sigma\tilde{W}\|_F^2 - 2\operatorname{trace}\left(\Sigma\tilde{W} \right) + n \\ &= \|\Sigma\|_F^2 - 2\operatorname{trace}\left(\Sigma\tilde{W} \right) + n. \end{aligned}$$

Thus, we need to maximize $\operatorname{trace}\left(\Sigma\tilde{W}\right)$. But this is maximized by $\tilde{W} = I$ by (1). Thus, the best approximating matrix is $W = UV^T$.

6 The "Thin" SVD

Also called "economy size" SVD. If $A \in \mathbb{C}^{m\times n}$, $A = U\Sigma V^T$, and $m \geq n$, then the "thin" SVD is $A = U_1\Sigma_1 V^T$ where

$$U_1 = [u_1, \ldots, u_n] \in \mathbb{C}^{m\times n}$$

and

$$\Sigma_1 = \operatorname{diag}(\sigma_1, \ldots, \sigma_n) \in \mathbb{R}^{n\times n}.$$

7 Applications of the SVD

1. Determining range, null space and rank (also numerical rank).

2. Matrix approximation.

3. Inverse and Pseudo-inverse: If $A = U\Sigma V^T$ and Σ is full rank, then $A^{-1} = V\Sigma^{-1}U^T$. If Σ is singular, then its pseudo-inverse is given by $A^\dagger = V\Sigma^\dagger U^T$, where $\Sigma^\dagger$ is formed by replacing every nonzero entry by its reciprocal.

4. Least squares: If we need to solve $Ax = b$ in the least-squares sense, then $x_{LS} = V\Sigma^{\dagger}U^T b$.

5. De-noising – Small singular values typically correspond to noise. Take the matrix whose columns are the signals, compute SVD, zero small singular values, and reconstruct.

6. Compression – We have signals as the columns of the matrix S, that is, the i signal is given by

$$S_i = \sum_{i=1}^{r} (\sigma_j v_{ij})\, u_j.$$

If some of the σ_i are small, we can discard them with small error, thus obtaining a compressed representation of each signal. We have to keep the coefficients $\sigma_j v_{ij}$ for each signal and the dictionary, that is, the vectors u_i that correspond to the retained coefficients.

8 Differences between SVD and eigen-decomposition

1. Not every matrix has an eigen-decomposition (not even any square matrix). Any matrix (even rectangular) has an SVD.
2. In eigen-decomposition $A = X\Lambda X^{-1}$, that is, the eigen-basis is not always orthogonal. The basis of singular vectors is always orthogonal.
3. In SVD we have two singular-bases (right and left).
4. SVD tells everything on a matrix.
5. SVD as no numerical problems.
6. Relation to condition number; the numerical problems with eigen-decomposition; multiplication by an orthogonal matrix is perfectly conditioned.

9 Linear regression in the least-squared loss

In Linear regression we aim to find the best linear approximation to a set of observed data. For the m data points $\{x_1, \ldots, x_m\}$, $x_i \in \mathbb{R}^n$, each receiving the value y_i, we look for the weight vector w that minimizes:

$$\sum_{i=1}^{n} (x_i^T w - y_i)^2 = \|Aw - y\|_2^2$$

Where A is a matrix that holds the data points as rows $A_i = x_i^T$.

Proposition 9.1. *The vector w that minimizes $\|Aw - y\|_2^2$ is $w = A^{\dagger}y = V\Sigma^{\dagger}U^T y$ for $A = U\Sigma V^T$ and $\Sigma^{\dagger}_{ii} = 1/\Sigma_{ii}$ if $\Sigma_{ii} > 0$ and 0 else.*

Let us define $U_{\|}$ and $U_{\perp}$ as the parts of U corresponding to positive and zero singular values of A respectively. Also let $y_{\|} = 0$ and $y_{\perp}$ be two vectors such that $y = y_{\|} + y_{\perp}$ and $U_{\|} y_{\perp} = 0$ and $U_{\perp} y_{\|} = 0$.

Since $y_{\|}$ and $y_{\perp}$ are orthogonal we have that $\|Aw - y\|_2^2 = \|Aw - y_{\|} - y_{\perp}\|_2^2 = \|Aw - y_{\|}\|_2^2 + \|y_{\perp}\|_2^2$. Now, since $y_{\|}$ is in the range of A there is a solution w for which $\|Aw - y_{\|}\|_2^2 = 0$. Namely, $w = A^{\dagger}y = V\Sigma^{\dagger}U^T y$ for $A = U\Sigma V^T$. This is because $U\Sigma V^T V\Sigma^{\dagger}U^T y = y_{\|}$. Moreover, we get that the minimal cost is exactly $\|y_{\perp}\|_2^2$ which is independent of w.

10 Optimal squared loss dimension reduction

Given a set of n vectors $x_1, \ldots, x_n$ in $\mathbb{R}^m$. We look for a rank k projection matrix $P \in \mathbb{R}^{m \times m}$ that minimizes:

$$\sum_{i=1} ||Px_i - x_i||_2^2$$

If we denote by A the matrix whose i'th column is x_i then this is equivalent to minimizing $||PA - A||_{Fro}^2$ Since the best possible rank k approximation to the matrix A is $A_k = \sum_{i=1}^{k} \sigma_i u_i v_i^T$ the best possible solution would be a projection P for which $PA = A_k$. This is achieved by $P = U_k U_k^T$ where U_k is the matrix corresponding to the first k left singular vectors of A.

If we define $y_i = U_k^T x_i$ we see that the values of $y_i \in \mathbb{R}^k$ are optimally fitted to the set of points x_i in the sense that they minimize:

$$\min_{y_1,\ldots,y_n} \min_{\Psi \in \mathbb{R}^{k \times m}} \sum_{i=1} ||\Psi y_i - x_i||_2^2$$

The mapping of $x_i \to U_k^T x_i = y_i$ thus reduces the dimension of any set of points $x_1, \ldots, x_n$ in $\mathbb{R}^m$ to a set of points $y_1, \ldots, y_n$ in $\mathbb{R}^k$ optimally in the squared loss sense. This is commonly referred to as Principal Component Analysis (PCA).