Optimization and Computational Linear Algebra for Data Science
Lecture 7: Singular value decomposition

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Warning: *This material is not meant to be lecture notes. It only gathers the main concepts and results from the lecture, without any additional explanation, motivation, examples, figures...*

1 The Spectral Theorem

The main result of this section is the following "Spectral Theorem" which tells us that a symmetric matrix is diagonalizable in an orthonormal basis.

Theorem 1.1 (*Spectral Theorem*)

Let $A \in \mathbb{R}^{n \times n}$ be a ***symmetric*** *matrix. Then there is a orthonormal basis of $\mathbb{R}^n$ composed of eigenvectors of A.*

Given an $n \times n$ symmetric matrix A, Theorem 1.1 tells us that one can find an orthonormal basis $(v_1, \dots, v_n)$ of $\mathbb{R}^n$ and scalars $\lambda_1, \dots, \lambda_n \in \mathbb{R}$ such that for all $i \in \{1, \dots, n\}$,

$$Av_i = \lambda_i v_i.$$

Let P be the $n \times n$ matrix whose columns are $v_1, \dots, v_n$. Since $(v_1, \dots, v_n)$ is an orthonormal basis, we get that P is an orthogonal matrix. Let $D = \mathrm{Diag}(\lambda_1, \dots, \lambda_n)$ and compute

$$AP = A \begin{pmatrix} | & | & & | \\ v_1 & v_2 & \cdots & v_n \\ | & | & & | \end{pmatrix} = \begin{pmatrix} | & | & & | \\ Av_1 & Av_2 & \cdots & Av_n \\ | & | & & | \end{pmatrix} = \begin{pmatrix} | & | & & | \\ \lambda_1 v_1 & \lambda_2 v_2 & \cdots & \lambda_n v_n \\ | & | & & | \end{pmatrix} = PD.$$

By multiplying by $P^\top$ on both sides, we get $APP^\top = PDP^\top$. Recall now that P is orthogonal, therefore $PP^\top = \mathrm{Id}_n$. We conclude that $A = PDP^\top$.

Theorem 1.2 (*Spectral Theorem, matrix formulation*)

Let $A \in \mathbb{R}^{n \times n}$ be a symmetric matrix. Then there exists an orthogonal matrix P and a diagonal matrix D of sizes $n \times n$, such that

$$A = PDP^\top.$$

Proposition 1.1

Let A be a $n \times n$ symmetric matrix and let $\lambda_1 \geq \dots \geq \lambda_n$ be its n eigenvalues and $v_1, \dots, v_n$ be the associated orthonormal family of eigenvectors. Then

$$v_1 = \operatorname*{arg\,max}_{\|v\|=1} v^\top A v\,, \qquad \text{and for } k = 2, \dots n, \qquad v_k = \operatorname*{arg\,max}_{\|v\|=1,\, v \perp v_1, \dots, v_{k-1}} v^\top A v.$$

Remark 1.1. *Applying the proposition above to the matrix $-A$ which is symmetric with eigenvalues $-\lambda_n \geq \dots \geq -\lambda_1$ and associated eigenvectors $v_n, \dots, v_1$, we get*

$$v_n = \operatorname*{arg\,min}_{\|v\|=1} v^\top A v\,, \qquad \text{and for } k = 1, \dots, n-1 \qquad v_k = \operatorname*{arg\,min}_{\|v\|=1,\, v \perp v_{k+1}, \dots, v_n} v^\top A v.$$

Positive matrices

Definition 1.1

A symmetric matrix $A \in \mathbb{R}^{n\times n}$ is said to be positive semi-definite *if*

$$\forall x \in \mathbb{R}^n,\ x^\top A x \geq 0. \tag{1}$$

The matrix A is said to be positive definite *if moreover the inequality in (1) is strict for all $x \neq 0$.*

Remark 1.2. *Negative semi-definite and negative definite matrices are defined analogously.*

Proposition 1.2

Let $A \in \mathbb{R}^{n\times n}$ be a symmetric matrix, and let $\lambda_1, \dots, \lambda_n \in \mathbb{R}$ its eigenvalues. Then

$$A \text{ is positive semi-definite} \iff \lambda_i \geq 0 \text{ for } i = 1, \dots, n,$$

and

$$A \text{ is positive definite} \iff \lambda_i > 0 \text{ for } i = 1, \dots, n.$$

Exercise 1.1. *Let $A \in \mathbb{R}^{n\times n}$.*

a. *Show that $A^\top A$ positive semi-definite.*

b. *Let M be a $n \times n$ symmetric positive semi-definite matrix. Show that there exists $A \in \mathbb{R}^{n\times n}$ such that $M = A^\top A$.*

2 Singular value decomposition

Theorem 2.1 (*Singular value decomposition (SVD)*)

Let $A \in \mathbb{R}^{n\times m}$. Then there exists two orthogonal matrices $U \in \mathbb{R}^{n\times n}$ and $V \in \mathbb{R}^{m\times m}$ and a matrix $\Sigma \in \mathbb{R}^{n\times m}$ such that $\Sigma_{1,1} \geq \Sigma_{2,2} \geq \cdots \geq 0$ and $\Sigma_{i,j} = 0$ for $i \neq j$

$$A = U\Sigma V^\top.$$

The columns $u_1, \dots, u_n$ of U (respectively the columns $v_1, \dots, v_m$ of V) are called the left (resp. right) singular vectors of A. The non-negative numbers $\Sigma_{i,i}$ are the singular values of A. Moreover $\mathrm{rank}(A) = \#\{i \,|\, \Sigma_{i,i} \neq 0\}$.

Notice that the singular vectors (similarly to the eigenvectors) are not uniquely defined: if $A = U\Sigma V^\top$ is a SVD of A, then $A = (-U)\Sigma(-V)^\top$ is also a SVD of A. However, with a slight abuse of language, we will often refer v_i as the i^{th} right singular vector of A.

2.1 Properties of the SVD

Let $A \in \mathbb{R}^{n\times m}$ and let $U\Sigma V^\top$ be a singular value decomposition of A as in Theorem 2.1. Let $u_1, \dots, u_n$ be the left singular vectors (i.e. the columns of U) and $v_1, \dots, v_m$ be the right singular vectors (i.e. the columns of V). Let $\sigma_i = \Sigma_{i,i}$ be the singular values of A.

Proposition 2.1

For $i = 1, \dots, \mathrm{rank}(A)$ we have

$$Av_i = \sigma_i u_i \qquad \textit{and} \qquad A^\top u_i = \sigma_i v_i.$$

The most important property of the singular vectors for us is the following:

Proposition 2.2

We have

$$v_1 = \operatorname*{arg\,max}_{\|v\|=1} \|Av\| \qquad \textit{and} \qquad \sigma_1 = \max_{\|v\|=1} \|Av\|. \tag{2}$$

It holds also that

$$v_2 = \operatorname*{arg\,max}_{\|v\|=1,\, v\perp v_1} \|Av\| \qquad \textit{and} \qquad \sigma_2 = \max_{\|v\|=1,\, v\perp v_1} \|Av\| \tag{3}$$

and more generally:

$$v_k = \operatorname*{arg\,max}_{\|v\|=1,\, v\perp v_1,\dots,v_{k-1}} \|Av\|. \qquad \textit{and} \qquad \sigma_k = \max_{\|v\|=1,\, v\perp v_1,\dots,v_{k-1}} \|Av\|. \tag{4}$$

Remark 2.1. *Considering $A^\top$ leads to an analogous result for the left singular vectors u_k:*

$$u_k = \operatorname*{arg\,max}_{\|u\|=1,\, u\perp u_1,\dots,u_{k-1}} \|A^\top u\|. \qquad \textit{and} \qquad \sigma_k = \max_{\|u\|=1,\, u\perp u_1,\dots,u_{k-1}} \|A^\top u\|. \tag{5}$$

Proof. Compute $A^\top A = V\Sigma^\top \Sigma V^\top = VDV^\top$ where the matrix $D \stackrel{\text{def}}{=} \Sigma^\top \Sigma$ is diagonal with $D_{i,i} = \sigma_i^2$. The family $(v_1, \dots, v_m)$ is therefore an orthonormal family of eigenvectors of the symmetric matrix $A^\top A$ and $\sigma_1^2 \geq \cdot \geq \sigma_m^2$ are the corresponding eigenvalues. The result follows then from Proposition 1.1 applied to $A^\top A$, noticing that $v^\top A^\top A v = \|Av\|^2$. □

2.2 Proof of Theorem 2.1

We apply the Spectral Theorem (Theorem 1.1) to the $m \times m$ matrix $A^\top A$: there exists an orthonormal basis $(v_1, \dots, v_m)$ of $\mathbb{R}^m$ of eigenvectors of $A^\top A$ associated to eigenvalues $\lambda_1 \geq \dots \geq \lambda_m$ that are all non-negative because $A^\top A$ is non-negative. Let $V \in \mathbb{R}^{m\times m}$ be the orthogonal matrix whose columns are $(v_1, \dots, v_m)$.

Let us write $\sigma_i = \sqrt{\lambda_i}$ and let $r = \max\{i | \sigma_i > 0\}$. Define for $i = 1, \dots, r$

$$u_i = \frac{1}{\sigma_i} A v_i \in \mathbb{R}^n. \tag{6}$$

Lemma 2.1

The family $(u_1, \dots, u_r)$ is orthonormal.

Proof. Let $i, j \in \{1, \dots, r\}$.

$$\langle u_i, u_j \rangle = \Big(\frac{1}{\sigma_i} A v_i\Big)^\top \Big(\frac{1}{\sigma_j} A v_j\Big) = \frac{1}{\sigma_i \sigma_j} v_i^\top A^\top A v_j = \frac{\sigma_i}{\sigma_j} v_i^\top v_j = \mathbb{1}_{i=j},$$

since $A^\top A v_i = \sigma_i^2 v_i$. □

If $r < n$ we let $(u_{r+1}, \dots, u_n)$ be an orthonormal family of vectors of $\mathbb{R}^n$ that are orthogonal to $u_1, \dots, u_r$. The family $(u_1, \dots, u_n)$ is then an orthonormal basis of $\mathbb{R}^n$ Let $U \in \mathbb{R}^{n\times n}$ be the orthogonal matrix whose columns are $(u_1, \dots, u_n)$.

Lemma 2.2

For $i = r+1, \dots, m$, $Av_i = 0$.

Proof. We compute for $i = r+1, \dots, m$:

$$\|Av_i\|^2 = v_i^\top A^\top A^\top v_i = v_i^\top (\lambda_i v_i) = \sigma_i^2 = 0.$$

□

Finally, we let $\Sigma \in \mathbb{R}^{n \times m}$ defined by:

$$\Sigma_{i,j} = \begin{cases} \sigma_i & \text{if} \quad i = j \\ 0 & \text{otherwise.} \end{cases}$$

It remains to verify that $A = U\Sigma V^\top$. Compute for $i = 1, \dots, m$, using the definition (6) and Lemma 2.2:

$$Av_i = \begin{cases} \sigma_i u_i & \text{if } i \leq r \\ 0 & \text{otherwise.} \end{cases}$$

By orthogonality of V and the construction of Σ one verify easily that

$$U\Sigma V^\top v_i = \begin{cases} \sigma_i u_i & \text{if } i \leq r \\ 0 & \text{otherwise.} \end{cases}$$

We conclude that for all $i \in \{1, \dots, m\}$, $Av_i = U\Sigma V^\top v_i$. Since a linear transformation is uniquely determined by the image of a basis, we conclude that $A = U\Sigma V^\top$.

It remains to show:

Lemma 2.3

$\text{rank}(A) = r$.

Proof. The family $(u_1, \dots, u_r)$ is orthonormal, hence linearly independent. By definition $u_i \in \text{Im}(A)$ which implies that $\text{rank}(A) = \dim(\text{Im}(A)) \geq r$. To prove the converse inequality, notice that by Lemma 2.2 $v_i \in \text{Ker}(A)$ for $i = r+1, \dots, m$. The vectors $(v_{r+1}, \dots, v_m)$ are orthonormal, hence linearly independent. This implies that $\dim(\text{Ker}(A)) \geq m - r$. We conclude by applying the rank Theorem:

$$\text{rank}(A) = m - \dim(\text{Ker}(A)) \leq m - (m - r) = r.$$

□

3 Interpretation of the SVD

3.1 Geometric interpretation

3.2 "Maximal variance" interpretation

Let $a_1, \dots, a_n \in \mathbb{R}^d$ be n points in d dimensions. We assume that this points are centered, meaning that

$$\sum_{i=1}^{n} a_i = 0.$$

Let A be the $n \times d$ matrix whose rows are $a_1, \dots, a_n$ and let $(v_1, \dots, v_n)$ be its right singular vectors. By Proposition 2.2, v_1, the first right singular vector of A, maximizes

$$v \mapsto \|Av\|^2 = \sum_{i=1}^{n} \langle a_i, v \rangle^2$$

over the unit sphere. This quantity is the variance of the coordinates of the points $a_1, \dots, a_n$ along the direction $\mathrm{Span}(v)$.

The first right singular vector v_1 gives therefore the direction along which the variance of the data is maximal. Proposition 2.2 gives also that

$$v_k = \underset{\|v\|=1,\, v \perp v_1, \dots, v_{k-1}}{\arg\max} \|Av\|^2. \tag{7}$$

Hence v_2 gives the direction orthogonal to v_1 that maximizes the variance and so on...

3.3 Best-fitting subspace

Let $a_1, \dots, a_n \in \mathbb{R}^d$ be n points in d dimensions. We consider the problem of finding the k-dimensional subspace (for $k = 1, \dots, n$) that fits "the best" these n data points. By "best", we mean here the k-dimensional subspace S that minimize the sum of the square distances to the n points:

$$\text{minimize} \quad \sum_{i=1}^{n} d(a_i, S)^2 \quad \text{with respect to } S \text{ subspace of dimension } k. \tag{8}$$

Let A be the $n \times d$ matrix whose rows are $a_1, \dots, a_n$. The goal of this section is to prove:

Theorem 3.1

Let $v_1, \dots, v_n$ be right singular vectors of A. Then for all $k \in \{1, \dots, n\}$, the subspace $\mathrm{Span}(v_1, \dots, v_k)$ is a solution of (8).

In this case we have for all $i \in \{1, \dots, n\}$,

$$d(a_i, S)^2 = \|a_i - P_S(a_i)\|^2 = \|a_i\|^2 - \|P_S(a_i)\|^2,$$

by Pythagorean Theorem (recall that $P_S(a_i) \perp (a_i - P_S(a_i))$). Since v_1 is of unit norm, $P_S(a_i) = \langle v_1, a_i \rangle v_1$, hence:

$$d(a_i, S)^2 = \|a_i\|^2 - \langle v_1, a_i \rangle^2.$$

Minimizing (8) is therefore equivalent to maximize

$$\sum_{i=1}^{n} \|P_S(a_i)\|^2. \tag{9}$$

Let us fix an orthonormal basis $(s_1, \dots, s_k)$ of S. Then for all $x \in \mathbb{R}^d$, $P_S(x) = \langle s_1, x \rangle s_1 + \cdots + \langle s_k, x \rangle s_k$, hence

$$\sum_{i=1}^{n} \|P_S(a_i)\|^2 = \sum_{i=1}^{n} \sum_{j=1}^{k} \langle a_i, s_j \rangle^2 = \|As_1\|^2 + \cdots + \|As_k\|^2, \tag{10}$$

Consequently, minimizing (8) is equivalent to maximizing (10) over all orthonormal families $(s_1, \dots, s_k)$.

For $k = 1$, Proposition 2.2 tells us that a subspace of dimension 1 that minimizes (8) is $\mathrm{Span}(v_1)$ because

$$v_1 = \arg\max_{\|v\|=1} \|Av\|. \tag{11}$$

If we now want to solve the problem for $k = 2$, a natural candidate for the subspace S would be $S = \mathrm{Span}(v_1, v_2)$ since by Proposition 2.2

$$v_2 = \arg\max_{\|v\|=1,\, v\perp v_1} \|Av\|. \tag{12}$$

We can follow this greedy strategy for $k = 3, \dots, n$, $S = \mathrm{Span}(v_1, \dots, v_k)$ is a natural candidate for being solution of (8).

It is not a priori obvious (except for $k = 1$) that $S = \mathrm{Span}(v_1, \dots, v_k)$ is a minimizer of (8) over all the subspaces of dimension k. We need the following lemma.

Lemma 3.1

Let $k \in \{2, \dots, k\}$. Assume that $(v_1, \dots, v_{k-1})$ is an orthonormal family that maximizes (10). Define

$$v_k = \arg\max_{\|v\|=1,\, v\perp \mathrm{Span}(v_1,\dots,v_{k-1})} \|Av\|.$$

Then $(v_1, \dots, v_k)$ is an orthonormal family and $\mathrm{Span}(v_1, \dots v_k)$ minimizes (8), i.e. $(v_1, \dots, v_k)$ maximizes (10).

Proof. Let S be a subspace of dimension k. Let $(w_1, \dots, w_k)$ be an orthonormal basis of S such that $w_k \perp \mathrm{Span}(v_1, \dots, v_{k-1})$. By definition of v_k, we have $\|Aw_k\| \leq \|Av_k\|$. We also assumed that $(v_1, \dots, v_k)$ maximizes (10), so

$$\|Av_1\|^2 + \cdots + \|Av_{k-1}\|^2 \geq \|Aw_1\|^2 + \cdots + \|Aw_{k-1}\|^2.$$

We conclude that

$$\|Av_1\|^2 + \cdots + \|Av_k\|^2 \geq \|Aw_1\|^2 + \cdots + \|Aw_k\|^2,$$

so $(v_1, \dots, v_k)$ maximizes (10). $\square$

Theorem 3.1 follows then by induction.