Singular Value Decomposition of Real Matrices

Jugal K. Verma

Indian Institute of Technology Bombay

Vivekananda Centenary College, 13 March 2020

Singular value decomposition of matrices

- **Theorem.** Let A be an $m \times n$ real matrix. Then $A = U\Sigma V^t$ where U is an $m \times m$ orthogonal matrix, V is an $n \times n$ orthogonal matrix and Σ is an $m \times n$ diagonal matrix whose diagonal entries are non-negative.

- The diagonal entries of Σ are called the **singular values of** A.
- The column vectors of V are called the **right singular vectors** of A
- The column vectors of V are called the **left singular vectors** of A.
- The equation $A = U\Sigma V^t$ is called a singular value decomposition of A.
- There are numerous applications of SVD. For example:
- Computation of bases of the four fundamental subspaces of A.
- Polar decomposition of square matrices
- Least squares approximation of vectors and data fitting
- Data compression
- Approximation of A by matrices of lower rank
- Computation of matrix norms

A brief history of SVD

- Eugenio Beltrami (1835-1899) and Camille Jordan (1838-1921) found the SVD for simplification of bilinear forms in 1870s.
- C. Jordan obtained geometric interpretation of the largest singular value
- J. J. Sylvester wrote two papers on the SVD in 1889.
- He found algorithms to diagonalise quadratic and bilinear forms by means of orthogonal substitutions.
- Erhard Schmidt (1876-1959) discovered the SVD for function spaces while investigating integral equations.
- His problem was to find the best rank k approximations to A of the form

$$u_1 v_1^t + \cdots + u_k v_k^t.$$

- Autonne found the SVD for complex matrices in 1913.
- Eckhart and Young extended SVD to rectangular matrices in 1936.
- Golub and Kahan introduced SVD in numerical analysis in 1965 .
- Golub proposed an algorithm for SVD in 1970.

Review of orthogonal matrices

- A real $n \times n$ matrix Q is called orthogonal if $Q^tQ = I$.
- A 2×2 orthogonal matrix has two possibilities:

$$A = \begin{bmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{bmatrix} \text{ or } B = \begin{bmatrix} \cos\theta & \sin\theta \\ \sin\theta & -\cos\theta \end{bmatrix}.$$

- The matrix A represents rotation of the plane by an angle of θ in anticlockwise direction.
- The matrix B represents a reflection with respect to $y = \tan(\theta/2)x$.
- **Definition.** A hyperplane in $\mathbb{R}^n$ is a subspace of dimension $n-1$.
- A linear transformation $T : \mathbb{R}^n \to \mathbb{R}^n$ is called a reflection with respect to a hyperplane H if $Tu = -u$ where $u \perp H$ and $Tu = u$ for all $u \in H$.
- **The Householder matrix for reflection.** Let u be a unit vector in $\mathbb{R}^n$.
- The Householder matrix of u, for reflection with respect to $L(u)^\perp$ is

$$H = I - 2uu^t.$$

- Then $Hu = u - 2u(u^tu) = -u$. If $w \perp u$ then $Hw = w - 2uu^tw = w$.
- So H induces reflection in the plane perpendicular to the line $L(u)$.
- Since $H = I - uu^t$, H is a symmetric and as $H^tH = I$, it is orthogonal.

Review of orthogonal matrices

- **Theorem.** (**Elié Cartan**) Any orthogonal $n \times n$ matrix is a product of atmost n Householder matrices.
- **Definition** [**Orthogonal Transformation**] Let V be a vector space with an inner product. A linear transformation $T : V \to V$ is called orthogonal if $\|Tu\| = \|u\|$ for all $u \in V$.
- **Theorem.** An orthogonal matrix is orthogonally similar to

$$\begin{bmatrix} I_r & & & & & & & \\ & \ddots & & & & & & \\ & & -I_s & & & & & \\ & & & \cos\theta_1 & -\sin\theta_1 & & & \\ & & & \sin\theta_1 & \cos\theta_1 & & & \\ & & & & & \ddots & & \\ & & & & & & \cos\theta_k & -\sin\theta_k \\ & & & & & & \sin\theta_k & \cos\theta_k \end{bmatrix}$$

Positive definite and positive semi-definite matrices

- **Definition.** A real symmetric matrix A is called positive definite (resp. positive semi-definite) if $x^tAx > 0$ (resp. $x^tAx \geq 0$) $\forall x \neq 0$.
- **Theorem.** Let A be an $n \times n$ real symmetric matrix. The A is positive definite if and only if each eigenvalue of A is positive.
- **Proof.** Let A be positive definite and x be an eigenvector with eigenvalue λ. Then $Ax = \lambda x$. Hence $x^tAx = \lambda||x||^2$. Thus $\lambda > 0$.
- Conversely, let each eigenvalue of A be positive.
- Suppose that $\{v_1, v_2, \ldots, v_n\}$ is an orthonormal basis of eigenvectors with positive eigenvalues $\lambda_1, \ldots, \lambda_n$.
- Then any nonzero vector x can be written as $x = a_1v_1 + \cdots + a_nv_n$ where at least one $a_i \neq 0$. Then
$$x^tAx = x^t(a_1\lambda_1v_1 + \cdots + a_n\lambda_nv_n) = \sum_{i=1}^{n} \lambda_i a_i^2 > 0.$$
- **Theorem.** Let A be an $n \times n$ real symmetric matrix. Then A is positive definite if and only if all principal minors are positive definite.

Proof of existence of SVD

- **Theorem.** Let A be an $m \times n$ real matrix of rank r. Then there exist orthogonal matrices $U \in \mathbb{R}^{m\times m}$, $V \in \mathbb{R}^{n\times n}$ and a diagonal matrix $\Sigma \in \mathbb{R}^{m\times n}$ with nonnegative diagonal entries $\sigma_1, \sigma_2, \ldots, \ldots$ such that

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

- **Proof.** Since Since A^tA is symmetric and positive semi-definite, there exists an $n \times n$ orthogonal matrix V whose column vectors are the eigenvectors of A^tA with non-negative eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_n$.
- Hence $A^tAv_i = \lambda_i v_i$ for $i = 1, 2, \ldots, n$. Let $r = \operatorname{rank} A$. Assume that
- $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_r > 0$ and $\lambda_j = 0$ for $j = r+1, r+2, \ldots, n$.
- Set $\sigma_i = \sqrt{\lambda_i}$ for all $i = 1, 2, \ldots, n$. Then $v_i^tA^tAv_i = \lambda_i v_i^t v_i = \lambda_i \geq 0$. Then $||Av_i|| = \sigma_i$ for $i = 1, 2, \ldots, n$. Set $Av_i/\sigma_i = u_i$.
- The set $u_1, u_2, \ldots, u_r$ is an orthonormal basis of $C(A)$.

$$u_i^t u_j = \frac{(Av_i)^t Av_j}{\sigma_i \sigma_j} = \frac{v_i^t v_j \lambda_j}{\sigma_i \sigma_j} = \delta_{ij}.$$

Proof of existence of SVD

- We can add to it an orthonormal basis $\{u_{r+1}, \ldots, u_m\}$ of $N(A^t)$ so that $U = [u_1, u_2, \ldots, u_m]$ is an orthogonal matrix.
- Since $Av_i = \sigma_i u_i$ for all i, we have the singular value decomposition

$$A = U\Sigma V^t \text{ where } \Sigma = \text{diag}\,(\sigma_1, \sigma_2, \ldots, \sigma_r, 0, 0, \ldots, 0).$$

- **Theorem.** Let A be an $m \times n$ real matrix. Then the largest singular value of A is given by

$$\sigma_1 = \max\{||Ax|| : x \in S^{n-1}\}$$

- **Proof.** Let $v_1, \ldots, v_n$ be an orthonormal basis of $\mathbb{R}^n$ consisting of e.vectors of A^tA with eigenvalues $\sigma_1^2 \geq \sigma_2^2 \geq \cdots \geq \sigma_r^2 > 0 \geq \cdots \geq 0$.
- Write $x = c_1v_1 + c_2v_2 + \cdots + c_nv_n$ for $c_1, \ldots, c_n \in \mathbb{R}$. Hence

$$||Ax||^2 = x^tA^tAx = x.(c_1\sigma_1^2v_1 + \cdots + c_r\sigma_r^2v_r) = c_1^2\sigma_1^2 + \cdots + c_r^2\sigma_r^2.$$

- Therefore $||Ax||^2 \leq \sigma_1^2(c_1^2 + c_2^2 + \cdots + c_n^2) \leq \sigma_1^2$ if $||x|| = 1$.
- The equality holds if $x = v_1$.

Polar decomposition and data compression

- **Theorem.** **(Polar decomposition of matrices.)** Let A be an $n \times n$ real matrix. Then $A = US$. where U is orthogonal and S is positive semi-definite.
- **Proof.** Let $A = U\Sigma V^t$ be a singular value decomposition of A.
- Then $A = UV^t(V\Sigma V^t)$. The matrix UV^t is orthogonal.
- Since the entries of Σ are nonnegative, $V\Sigma V^t$ is a positive semi-definite.
- **Use of SVD in image processing.** Suppose that a picture consists of 1000×1000 array of pixels. This can be thought of a 1000×1000 matrix A of numbers which represent colors.
- Suppose $A = U\Sigma V^t$. Then can be written as a sum of rank one matrices:
$$A = \sigma_1 u_1 v_1^t + \sigma_2 u_2 v_2^t + \cdots + \sigma_r u_r v_r^t.$$
- Suppose that we take 20 singular values. Then we send $20 \times 2000 = 40000$ numbers rather than a million numbers.
- This represents a compression of $25 : 1$.

Least squares approximation

- Consider a system of linear equations $Ax = b$
- where A is an $m \times n$ real matrix, x is an unknown vector and $b \in \mathbb{R}^m$.
- If $b \in C(A)$ then we use Gauss elimination to find x.
- Otherwise we try to find x so that $||Ax - b||$ is smallest.
- To find such an x, we project b in the column space of A.
- Therefore $Ax - b \in C(A)^{\perp}$. Hence $A^t(Ax - b) = 0$. So

$$A^tAx = A^tb.$$

- These are called the **normal equations.**
- Let $A = U\Sigma V^t$ be an SVD for A. Then
$$Ax - b = U\Sigma V^t x - b = U\Sigma V^t x - UU^t b = U(\Sigma V^t x - U^t b).$$
- Set $y = V^t x, c = U^t b$. As U is orthogonal $||Ax - b|| = ||\Sigma y - c||$.
- Let $y = (y_1, y_2, \ldots, y_m)^t$ and $c = U^t b = (c_1, c_2, \ldots, c_m)^t$. Then
$$\Sigma y - c = (\sigma_1 y_1 - c_1, \sigma_2 y_2 - c_2, \ldots \sigma_r y_r - c_r, -c_{r+1}, \ldots, c_m)^t$$
- So Ax is the best approximation to $b \iff \sigma_i y_i = c_i$ for $i = 1, \ldots, r$.

Data fitting

- Suppose we have a large number of data points $(x_i, y_i),\ i = 1, 2, \ldots, n$ collected from some experiment. Sometime we believe that these points should lie on a straight line. So we want a linear function
$$y(x) = s + tx \text{ such that } y(x_i) = y_i,\ i = 1, \ldots, n'.$$
- Due to uncertainity in data and experimental error, in practice the points will deviate somewhat from a straightline and so it is impossible to find a linear $y(x)$ that passes through all of them.
- So we seek a line that fits the data well, in the sense that the errors are made as small as possible. A natural question that arises now is: how do we define the error?
- Consider the following system of linear equations, in the variables s and t, and known coefficients $x_i, y_i,\ i = 1, \ldots, n$:

$$y_1 = s + x_1 t,\quad y_2 = s + x_2 t \quad \ldots \quad y_n = s + x_n t$$

Data fitting

- Note that typically n would be much greater than 2. If we can find s and t to satisfy all these equations, then we have solved our problem. However, for reasons mentioned above, this is not always possible.
- For given values of s and t the error in the ith equation is $|y_i - s - x_i t|$. There are several ways of combining the errors in the individual equations to get a measure of the total error.
- The following are three examples:

$$\sqrt{\sum_{i=1}^{n}(y_i - s - x_i t)^2}, \quad \sum_{i=1}^{n}|y_i - s - x_i t|, \quad \max{}_{1\le i\le n}\, |y_i - s - x_i t|.$$

- Both analytically and computationally, a nice theory exists for the first of these choices and this is what we shall study. The problem of finding s, t so as to minimize

$$\sqrt{\sum_{i=1}^{n}(y_i - s - x_i t)^2}$$

- is called a **least squares problem**.

- The problem can be written in terms of matrices as

$$A = \begin{bmatrix} 1 & x_1 \\ 1 & x_2 \\ . & . \\ . & . \\ 1 & x_n \end{bmatrix}, \; b = \begin{bmatrix} y_1 \\ y_2 \\ . \\ . \\ y_n \end{bmatrix}, \text{ and } x = \begin{bmatrix} s \\ t \end{bmatrix}, \text{ so that } Ax = \begin{bmatrix} s + tx_1 \\ s + tx_2 \\ . \\ . \\ s + tx_n \end{bmatrix}.$$

- The least squares problem is finding an x such that $||b - Ax||$ is minimized, i.e., find an x such that Ax is the best approximation to b in the column space of A.
- This is precisely the problem of finding x such that $b - Ax$ is orthogonal to the column space of A.
- A straight line can be considered as a polynomial of degree 1. We can also try to fit an mth degree polynomial

$$y(x) = s_0 + s_1 x + s_2 x^2 + \cdots + s_m x^m$$

- to the data points $(x_i, y_i), \; i = 1, \ldots, n$, so as to minimize the error. In this case $s_0, s_1, \ldots, s_m$ are the variables and we have

$$A = \begin{pmatrix} 1 & x_1 & x_1^2 & . & . & x_1^m \\ 1 & x_2 & x_2^2 & . & . & x_2^m \\ & . & . & . & . & . \\ & . & . & . & . & . \\ 1 & x_n & x_n^2 & . & . & x_n^m \end{pmatrix}, \; b = \begin{pmatrix} y_1 \\ y_2 \\ . \\ . \\ y_n \end{pmatrix}, \; x = \begin{pmatrix} s_0 \\ s_1 \\ . \\ . \\ s_m \end{pmatrix}.$$

- Example: Find s, t such that the straight line $y = s + tx$ best fits the following data in the least squares sense:

$$y = 1 \text{ at } x = -1, \quad y = 1 \text{ at } x = 1, \quad y = 3 \text{ at } x = 2.$$

- We want to project $b = (1, 1, 3)^t$ onto the column space of $A = \begin{pmatrix} 1 & -1 \\ 1 & 1 \\ 1 & 2 \end{pmatrix}$.

  Now $A^t A = \begin{pmatrix} 3 & 2 \\ 2 & 6 \end{pmatrix}$ and $A^t b = \begin{pmatrix} 5 \\ 6 \end{pmatrix}$.
- The normal equations are $\begin{pmatrix} 3 & 2 \\ 2 & 6 \end{pmatrix} \begin{pmatrix} s \\ t \end{pmatrix} = \begin{pmatrix} 5 \\ 6 \end{pmatrix}$.
- The solution is $s = 9/7, \; t = 4/7$ and the best line is $y = \frac{9}{7} + \frac{4}{7}x$.

Approximation of a matrix by lower rank matrices

- A matrix norm on the space $V = \mathbb{R}^{m\times n}$ is a function $f : \mathbb{R}^{m\times n} \to \mathbb{R}$ which satisfies the following conditions for all $A, B \in V$ and $r \in R$,
- (1) $f(A) \geq 0$ and $f(A) = 0$ if and only if $A = 0$.
  (2) $f(A+B) \leq f(A) + f(B)$
  (3) $f(rA) = |r|f(A)$.
- Matrix norms are constructed using vector norms. If $v = (v_1, v_2, \ldots, v_n) \in \mathbb{R}^n$ then the p norm of v is defined as
$$||v||_p = \sqrt[p]{|v_1|^p + \cdots + |v_n|^p}.$$
- The infinity norm is defined as $||v||_\infty = \max\{|v_1|, |v_2|, \ldots, |v_n|\}$.
- **Example.** (1) The Frobenius norm of $A \in \mathbb{R}^{m\times n}$ is defined as
$$||A||_F = \sqrt{\sum_{i,j} |a_{ij}|^2}.$$
- One can show that $||A||_F = \sqrt{\mathrm{Tr}(AA^t)} = \sqrt{\sigma_1^2 + \cdots + \sigma_r^2}$.
- (2) Let p be a positive integer. Then $||A||_p = \sup_{x\neq 0} \frac{||Ax||_p}{||x||_p}$.
- We shall denote the 2-norm of A simply by $||A||$.

Low rank approximations

- **Theorem.** **[Eckhart-Young, 1936]** Let $A \in \mathbb{R}^{m\times n}$ and $\text{rank}(A) = r$. Let $A = U\Sigma V^t$ be a singular value decomposition of A with singular values
$$\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_r > 0.$$
- Let $A_k = \sum_{i=1}^{k} \sigma_i u_i v_i^t$. Then $\min_{\text{rank}(B)=k} ||A - B|| = ||A - A_k|| = \sigma_{k+1}$.
- **Proof.** Since $A_k = U\text{diag}(\sigma_1, \sigma_2, \ldots, \sigma_k, 0, \ldots, 0)V^t$, $\text{rank}(A_k) = k$.
- Note that $U^tAV - U^tA_kV = \text{diag}(0, \ldots, 0, \sigma_{k+1}, \ldots, \sigma_r, 0, \ldots, 0)$.
- Hence $||A - A_k|| = ||U^t(A - A_k)V|| = \sigma_{k+1}$.
- Let $B \in \mathbb{R}^{m\times n}$ be a rank k matrix. Since $\dim N(B) = n - k$,
- We can choose an orthonormal basis $\{x_1, x_2, \ldots, x_{n-k}\}$ of $N(B)$.
- Therefore $W = L(v_1, v_2, \ldots, v_{k+1}) \cap N(B) \neq 0$.
- Let z be a unit vector in $W \cap N(B)$. Then $Bz = 0$ and
$$Az = \sum_{i=1}^{r} \sigma_i u_i v_i^t z = \sum_{i=1}^{k+1} \sigma_i (v_i^t z) u_i$$
- Hence $||A - B||^2 \geq ||Az - Bz||^2 = ||Az||^2 = \sum_{i=1}^{k+1} \sigma_i^2 (v_i^t z)^2 \geq \sigma_{k+1}^2$.
- Thus A_k is closest to A among rank k matrices.

References

1. S. Axler, *Linear algebra done right,* III edition, Springer, 2015.
2. Gilbert Strang, *Linear Algebra and its Applications.* Indian edition, 2020.
3. G. W. Stewart, *On the early history of the singular value decomposition,* SIAM Review **35** (1993),551-566.