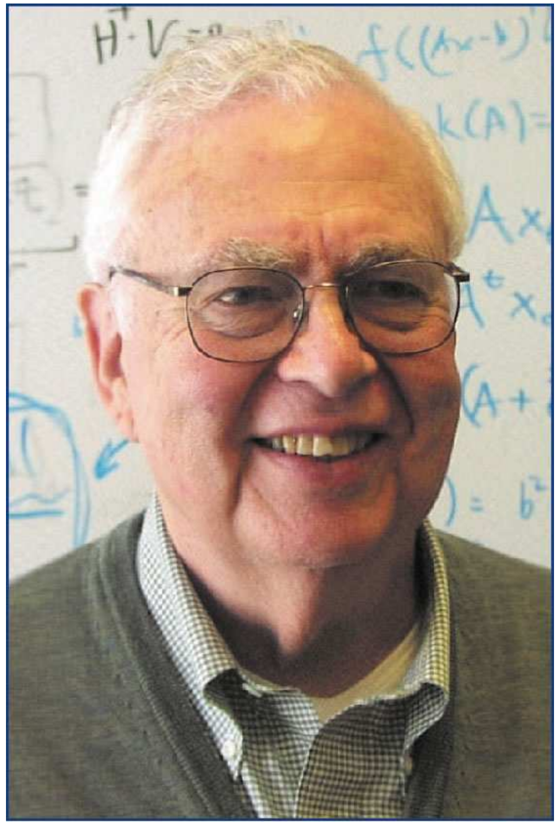
Lecture 8: The SV Decomposition



Singular values

Theorem. Let $O \neq A \in \mathbb{C}_r^{m\times n}$, let $\sigma(A)$, the **singular values** of A, be

$$\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_r > 0 \ , \tag{1}$$

let $\{\mathbf{u}_1, \mathbf{u}_2, \ldots, \mathbf{u}_r\}$ be an **o.n. set of eigenvectors** of AA^* corresponding to its **nonzero eigenvalues**:

$$AA^*\mathbf{u}_i = \sigma_i^2 \mathbf{u}_i \ , \quad i \in \overline{1,r} \tag{2a}$$

$$\langle \mathbf{u}_i, \mathbf{u}_j \rangle = \delta_{ij} \ , \quad i,j \in \overline{1,r} \ , \tag{2b}$$

and let $\{\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_r\}$ be defined by

$$\mathbf{v}_i = \frac{1}{\sigma_i} A^*\mathbf{u}_i \ , \quad i \in \overline{1,r} \ . \tag{3}$$

Then $\{\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_r\}$ is an **o.n. set of eigenvectors** of A^*A corresponding to its nonzero eigenvalues

$$A^*A\mathbf{v}_i = \sigma_i^2 \mathbf{v}_i \ , \quad i \in \overline{1,r} \tag{4a}$$

$$\langle \mathbf{v}_i, \mathbf{v}_j \rangle = \delta_{ij} \ , \quad i,j \in \overline{1,r} \ . \tag{4b}$$

Singular values (cont'd)

Furthermore,

$$\mathbf{u}_i = \frac{1}{\sigma_i} A\mathbf{v}_i \ , \quad i \in \overline{1, r} \ . \tag{5}$$

Dually, let the vectors $\{\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_r\}$ satisfy (4a)–(4b) and let the vectors $\{\mathbf{u}_1, \mathbf{u}_2, \ldots, \mathbf{u}_r\}$ be defined by (5). Then $\{\mathbf{u}_1, \mathbf{u}_2, \ldots, \mathbf{u}_r\}$ satisfy (2a) and (2b). $\square$

Singular values (cont'd)

Furthermore,

$$\mathbf{u}_i = \frac{1}{\sigma_i} A\mathbf{v}_i \ , \quad i \in \overline{1, r} \ . \tag{5}$$

Dually, let the vectors $\{\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_r\}$ satisfy (4a)–(4b) and let the vectors $\{\mathbf{u}_1, \mathbf{u}_2, \ldots, \mathbf{u}_r\}$ be defined by (5). Then $\{\mathbf{u}_1, \mathbf{u}_2, \ldots, \mathbf{u}_r\}$ satisfy (2a) and (2b). $\square$

Notes.

(a) A and A^* have the same singular values.

(b) Singular values are **unitarily invariant**.

Proof. Let $A \in \mathbb{C}^{m\times n}$, and let $U \in U^{m\times m}$, $V \in U^{n\times n}$ be unitary. Then

$$(UAV)(UAV)^* = UAVV^*A^*U^* = UAA^*U^*$$

is similar to AA^*, and therefore has the same eigenvalues. Therefore UAV and A have the same singular values.

Singular values (cont'd)

(c) (**Lanczos**) Let $A \in \mathbb{C}_r^{m\times n}$. Then $\begin{bmatrix} O & A \\ A^* & O \end{bmatrix}$ has $2r$ nonzero eigenvalues given by $\pm\,\sigma_j(A)$, $j \in \overline{1,r}$.

Singular values (cont'd)

(c) (**Lanczos**) Let $A \in \mathbb{C}_r^{m\times n}$. Then $\begin{bmatrix} O & A \\ A^* & O \end{bmatrix}$ has $2r$ nonzero eigenvalues given by $\pm\,\sigma_j(A)$, $j \in \overline{1,r}$.

(d) **An extremal characterization**. Let $A \in \mathbb{C}_r^{m\times n}$. Then

$$\sigma_k(A) = \max\{\|A\mathbf{x}\| : \|\mathbf{x}\| = 1, \mathbf{x} \perp \mathbf{x}_1, \dots, \mathbf{x}_{k-1}\}, \quad k \in \overline{1,r}, \quad (1)$$

where $\|\ \|$ denotes the Euclidean norm, and

$\{\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_{k-1}\}$ is an o.n. set of vectors in $\mathbb{C}^n$, defined by

$$\|A\mathbf{x}_1\| = \max\{\|A\mathbf{x}\| : \|\mathbf{x}\| = 1\}$$

$$\|A\mathbf{x}_j\| = \max\{\|A\mathbf{x}\| : \|\mathbf{x}\| = 1, \mathbf{x} \perp \mathbf{x}_1, \dots, \mathbf{x}_{j-1}\}, \quad j = 2, \dots, k-1$$

and RHS(1) is the (attained) supremum of $\|A\mathbf{x}\|$ over all vectors $\mathbf{x} \in \mathbb{C}^n$ with norm one, which are perpendicular to $\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_{k-1}$.

Singular values (cont'd)

(e) **A condition number**. Let A be nonsingular, and consider the sensitivity of the solution of

$$A\mathbf{x} = \mathbf{b} \tag{1}$$

to changes in the vector $\mathbf{b}$. Changing $\mathbf{b}$ to $(\mathbf{b} + \delta\mathbf{b})$ results in a change of the solution $\mathbf{x} = A^{-1}\mathbf{b}$ to $\mathbf{x} + \delta\mathbf{x}$, with

$$\delta\mathbf{x} = A^{-1}\delta\mathbf{b}\ . \tag{2}$$

For any consistent pair of norms it follows from (1) that

$$\|\mathbf{b}\| \leq \|A\|\|\mathbf{x}\|$$

Similarly, from (2), $\quad \|\delta\mathbf{x}\| \leq \|A^{-1}\|\|\delta\mathbf{b}\|$

Therefore $\quad \dfrac{\|\delta\mathbf{x}\|}{\|\mathbf{x}\|} \leq \|A\|\|A^{-1}\|\dfrac{\|\delta\mathbf{b}\|}{\|\mathbf{b}\|} = \mathrm{cond}(A)\dfrac{\|\delta\mathbf{b}\|}{\|\mathbf{b}\|}$

where $\|A\|\|A^{-1}\|$, called the **condition number** of A, is denoted $\mathrm{cond}(A)$.

Singular values (cont'd)

The **spectral condition number** corresponding to the spectral norm is,

$$\operatorname{cond}(A) = \frac{\sigma_1(A)}{\sigma_n(A)} \ .$$

For this condition number, $\operatorname{cond}(A^*A) = (\operatorname{cond}(A))^2$.

(f) **Weyl's inequalities**. Let $A \in \mathbb{C}_r^{n\times n}$ have eigenvalues ordered by

$$|\lambda_1| \geq |\lambda_2| \geq \cdots \geq |\lambda_n|$$

and singular values

$$\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_r \ .$$

Then, for $k = 1, \ldots, r$,

$$\sum_{j=1}^{k} |\lambda_j| \leq \sum_{j=1}^{k} \sigma_j \ ,$$

$$\prod_{j=1}^{k} |\lambda_j| \leq \prod_{j=1}^{k} \sigma_j \ .$$

The SVD theorem

Theorem. Let $O \neq A \in \mathbb{C}_r^{m \times n}$, and let

$$\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_r > 0$$

be the singular values of A.

Then there exist unitary matrices $U \in U^{m \times m}$ and $V \in U^{n \times n}$ such that the matrix

$$\Sigma = U^* A V = \begin{bmatrix} \sigma_1 & & & \vdots & \\ & \ddots & & \vdots & O \\ & & \sigma_r & \vdots & \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ & O & & \vdots & O \end{bmatrix}$$

is diagonal.

SVD and the Moore–Penrose inverse

Theorem (Penrose). Let $A \in \mathbb{C}_r^{m\times n}$ have the SVD

$$A = U\Sigma V^*$$

with
$$\Sigma = \operatorname{diag}\,(\sigma_1, \cdots, \sigma_r, 0, \cdots, 0) \in \mathbb{R}^{m\times n}\ .$$

Then
$$A^\dagger = V\Sigma^\dagger U^*$$

where
$$\Sigma^\dagger = \operatorname{diag}\left(\frac{1}{\sigma_1}, \cdots, \frac{1}{\sigma_r}, 0, \cdots, 0\right) \in \mathbb{R}^{n\times m}\ .$$

A minimum property of the Moore–Penrose inverse. Let G be a $\{1\}$–inverse of $A \in \mathbb{C}_r^{m\times n}$ with singular values

$$\sigma_1(G) \geq \sigma_2(G) \geq \cdots \geq \sigma_s(G) \tag{1}$$

where $s = \operatorname{rank} G$ ($\geq$ $\operatorname{rank} A$). Then

$$\sigma_i(G) \ \geq\ \sigma_i(A^\dagger)\ , \quad i = 1, \ldots, r\ . \tag{2}$$

Truncation

Let $A \in \mathbb{C}_r^{m\times n}$ have the SVD $A = U\Sigma V^*$, and denote

$$U_{(k)} = \begin{bmatrix} \mathbf{u}_1 & \ldots & \mathbf{u}_k \end{bmatrix} \in \mathbb{C}^{m\times k}\ , \quad V_{(k)} = \begin{bmatrix} \mathbf{v}_1 & \ldots & \mathbf{v}_k \end{bmatrix} \in \mathbb{C}^{n\times k}\ ,$$

$$\Sigma_{(k)} = \begin{bmatrix} \sigma_1 & & \\ & \ddots & \\ & & \sigma_k \end{bmatrix} \in \mathbb{C}^{k\times k}\ .$$

$$\therefore\ \ A = \sum_{i=1}^{r} \sigma_i\, \mathbf{u}_i \mathbf{v}_i^* = U_{(r)}\Sigma_{(r)}V_{(r)}^*\ ,\quad A^\dagger = \sum_{i=1}^{r} \frac{1}{\sigma_i}\, \mathbf{v}_i \mathbf{u}_i^* = V_{(r)}\Sigma_{(r)}^{-1}U_{(r)}^*$$

For $1 \le k \le r$ we write, analogously,

$$A_{(k)} = \sum_{i=1}^{k} \sigma_i\, \mathbf{u}_i \mathbf{v}_i^* = U_{(k)}\Sigma_{(k)}V_{(k)}^* \in \mathbb{C}_k^{m\times n}\ .$$

In particular, $A = A_{(r)}$.

Best rank approximation

Definition. Given a matrix $A \in \mathbb{C}_r^{m\times n}$ and an integer k, $1 \le k \le r$, a **best rank-k approximation** of A is a matrix $X \in \mathbb{C}_k^{m\times n}$ satisfying

$$\|A - X\|_F = \inf_{Z \in \mathbb{C}_k^{m\times n}} \|A - Z\|_F \ .$$

Theorem (Schmidt approximation theorem). Let $A \in \mathbb{C}_r^{m\times n}$, and $1 \le k \le r$. Then **a best rank-k approximation** of A is

$$A_{(k)} = U_{(k)} \Sigma_{(k)} V_{(k)}^* \ ,$$

which is **unique** iff $\sigma_k \neq \sigma_{k+1}$.

The **approximation error** of $A_{(k)}$ is

$$\|A - A_{(k)}\|_F = \left(\sum_{i=k+1}^{r} \sigma_i^2 \right)^{1/2} \ .$$

TLS

Given a linear system

$$A\mathbf{x} = \mathbf{b}$$

the **least–squares problem** is to solve an approximate system

$$A\mathbf{x} = \widetilde{\mathbf{b}}$$

where $\widetilde{\mathbf{b}} \in R(A)$ minimizes

$$\|\widetilde{\mathbf{b}} - \mathbf{b}\|_2 \ .$$

The **total least–squares (TLS) problem** is to to solve an approximate system

$$\widetilde{A}\mathbf{x} = \widetilde{\mathbf{b}} \tag{1}$$

where $\widetilde{\mathbf{b}} \in R(\widetilde{A})$ and the pair $\{\widetilde{A}, \widetilde{\mathbf{b}}\}$ minimizes $\|[\widetilde{A} \vdots \widetilde{\mathbf{b}}] - [A \vdots \mathbf{b}]\|_F$.

Note that in the TLS problem, both the matrix A and the vector $\mathbf{b}$ are modified.

TLS (cont'd)

Since (1) is equivalent to

$$\begin{bmatrix} \mathbf{x} \\ -1 \end{bmatrix} \in N([\widetilde{A} \vdots \widetilde{\mathbf{b}}]) \ , \tag{2}$$

the **TLS problem** is:

$$\text{find } [\widetilde{A} \vdots \widetilde{\mathbf{b}}] \in \mathbb{C}^{m \times (n+1)}$$

so as to minimize,

$$\| [\widetilde{A} \vdots \widetilde{\mathbf{b}}] - [A \vdots \mathbf{b}] \|_F$$

subject to (2), for some $\mathbf{x}$.

TLS (cont'd)

Theorem. Let $A \in \mathbb{C}_n^{m \times n}$, let the system $A\mathbf{x} = \mathbf{b}$ be inconsistent, let $[A \vdots \mathbf{b}]$ have the SVD

$$[A \vdots \mathbf{b}] = U \Sigma V^* = \sum_{i=1}^{n+1} \sigma_i \, \mathbf{u}_i \mathbf{v}_i^* \ , \tag{1}$$

and let σ_k be the smallest singular value such that $\mathbf{v}_k$ has non–zero last component $\mathbf{v}_k[n+1]$. Then **a solution** of the TLS problem is

$$[\widetilde{A} \vdots \widetilde{\mathbf{b}}] = [A \vdots \mathbf{b}] - \sigma_k \, \mathbf{u}_k \mathbf{v}_k^* \tag{2}$$

and the **error of approximation** is

$$\| [\widetilde{A} \vdots \widetilde{\mathbf{b}}] - [A \vdots \mathbf{b}] \|_F = \sigma_k \ . \tag{3}$$

The solution (2) is unique iff the smallest singular value σ_k, as above, is unique.

Distance of $A \in \mathbb{C}_r^{m\times n}$ from $\mathbb{C}_k^{m\times n}$, $k \le r$

Let $O \neq A \in \mathbb{C}_r^{m\times n}$ have singular values

$$\sigma_1 \ge \sigma_2 \ge \cdots \ge \sigma_r > 0$$

and let

$$M_{r-1} = \bigcup_{k=0}^{r-1} \mathbb{C}_k^{m\times n} \tag{1}$$

be the **set of** $m \times n$ **matrices of rank** $\le r-1$. Then the **distance**, using either the Frobenius norm or the spectral norm, of A from M_{r-1} is

$$\inf_{X \in M_{r-1}} \|A - X\| = \sigma_r \ . \tag{2}$$

Distance of A from $\mathbb{C}_k^{m\times n}$, $k \le r$ (cont'd)

Two easy consequences of

$$\inf_{X\in M_{r-1}} \|A - X\| = \sigma_r \ . \tag{2}$$

are:

(a) Let A be as above, and let $B \in \mathbb{C}^{m\times n}$ satisfy $\|B\| < \sigma_r$; then $\operatorname{rank}(A+B) \ge \operatorname{rank} A$.

(b) For any $0 \le k \le \min\{m,n\}$, the $m \times n$ matrices of rank $\le k$ form a **closed set** in $\mathbb{C}^{m\times n}$.

In particular, the $n \times n$ singular matrices form a closed set in $\mathbb{C}^{n\times n}$. For any nonsingular $A \in \mathbb{C}^{n\times n}$ with singular values

$$\sigma_1 \ge \sigma_2 \ge \cdots \ge \sigma_n > 0$$

the **smallest singular value** σ_n is its **distance from singularity**.