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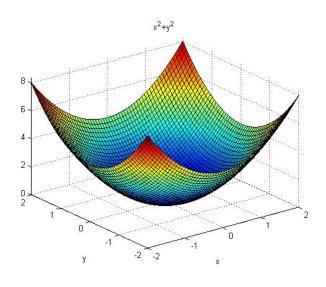
Positive Definite Matrices (正定矩阵)

6.3

SINGULAR VALUE DECOMPOSITION

(奇异值分解)

A^TA and AA^T
SVD Theorem
Applications



I. Facts about $A^{T}A$ and AA^{T} ($A \in \mathbb{R}^{m \times n}$)

- \Box rank $(A^{T}A)$ = rank (AA^{T}) = rank(A) = rank (A^{T}) = r.
- □ $A^{T}A$ and AA^{T} are real symmetric (degree n and m respectively), and positive semidefinite. ($A^{T}A$ and AA^{T} 的特征值为非负实数)
- \Box The eigenvalues of $A^{T}A$ and AA^{T} :
 - \square $A^{\mathsf{T}}A$ has *n* eigenvalues λ_1 , ..., λ_n , then

$$\lambda_1 \ge \lambda_2 \ge \dots \ge \lambda_r > 0 = \lambda_{r+1} = \dots = \lambda_n$$
.

 \square AA^{T} has m eigenvalues $\mu_1, ..., \mu_m$, then

$$\mu_1 \ge \mu_2 \ge \dots \ge \mu_r > 0 = \mu_{r+1} = \dots = \mu_m.$$

- □ We have the following conclusion: $\lambda_i = \mu_i > 0$, i = 1, ..., r. ($A^T A$ and AA^T 的非零特征值集合相同)
- **Definition**: $\sigma_i = \sqrt{\lambda_i} = \sqrt{\mu_i} > 0$ (i = 1, ..., r) are called the singular values (奇异值) of A.

Remark 若 A 是 $m \times n$ 矩阵, B是 $n \times m$ 矩阵, 且 $m \neq n$, 则 AB 与 BA 有相同的非零特征值.

Proof: 不妨假设 m > n, 一方面我们有:

$$\begin{bmatrix} I_m & \mathbf{0} \\ -\lambda^{-1}B_{n\times m} & I_n \end{bmatrix} \begin{bmatrix} \lambda I_m & A_{m\times n} \\ B_{n\times m} & I_n \end{bmatrix} = \begin{bmatrix} \lambda I_m & A \\ \mathbf{0} & I_n - \lambda^{-1}BA \end{bmatrix}$$

另一方面,

$$\begin{bmatrix} I_m & -A_{m\times n} \\ \mathbf{0} & I_n \end{bmatrix} \begin{bmatrix} \lambda I_m & A_{m\times n} \\ B_{n\times m} & I_n \end{bmatrix} = \begin{bmatrix} \lambda I_m - AB & \mathbf{0} \\ B & I_n \end{bmatrix}$$

对上两式两边同时取行列式有

$$\det\left(\begin{bmatrix} \lambda I_m & A \\ \mathbf{0} & I_n - \lambda^{-1} BA \end{bmatrix}\right) = \det\left(\begin{bmatrix} \lambda I_m - AB & \mathbf{0} \\ B & I_n \end{bmatrix}\right)$$

即

$$\lambda^{m}|I_{n} - \lambda^{-1} BA| = |\lambda I_{m} - AB|$$
$$|\lambda I_{m} - AB| = \lambda^{m-n}|\lambda I_{n} - BA|$$

故 AB 与 BA 有相同的非零特征值.

Example 1 Find the singular values of the following matrices:

$$(1) \mathbf{A} = \begin{bmatrix} 1 & 2 \\ 0 & 0 \\ 0 & 0 \end{bmatrix}; \qquad (2) \mathbf{A} = \begin{bmatrix} 0 & -1 & 1 \\ 2 & 0 & 0 \end{bmatrix}.$$

Solution

(1)
$$\mathbf{A}\mathbf{A}^{\mathrm{T}} = \begin{bmatrix} 5 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$
, so the eigenvalues of $\mathbf{A}\mathbf{A}^{\mathrm{T}}$ are 5, 0 and 0, and the singular value of \mathbf{A} is $\sqrt{5}$.

(We can also check the eigenvalues of $A^{T}A$)

(2) $\mathbf{A}\mathbf{A}^{\mathrm{T}} = \begin{bmatrix} 2 & 0 \\ 0 & 4 \end{bmatrix}$, so the eigenvalues of $\mathbf{A}\mathbf{A}^{\mathrm{T}}$ are 2 and 4, and the singular values of \mathbf{A} are $\sqrt{2}$ and 2.

II. Singular Value Decomposition (奇异值分解)

We have seen that any real *symmetric* matrix **A** can be factored into

$$\mathbf{A} = \mathbf{Q} \mathbf{\Lambda} \mathbf{Q}^{\mathrm{T}}$$
 (eigenvalue-eigenvector factorization),

where Q is orthogonal, and Λ is diagonal.

There is an extension of this result.

Theorem 1 Any $n \times n$ invertible real matrix can be factored into

$$A = Q_1 S Q_2^{\mathrm{T}},$$

(invertible) = (orthogonal) (positive definite diagonal) (orthogonal)

where Q_1 and Q_2 are *orthogonal* matrices of degree n, and S is a positive definite *diagonal* matrix of degree n.

Proof Since *A* is invertible, we have

$$\boldsymbol{A} = \boldsymbol{Q}_1 \boldsymbol{S} \boldsymbol{Q}_2^{\mathrm{T}}$$

$$x^{T}A^{T}Ax = (Ax)^{T}(Ax) = ||Ax||^{2} > 0$$
, for any $x \neq 0$,

so $A^{T}A$ is positive definite.

Thus there exists an orthogonal matrix Q_2 , such that

$$\mathbf{Q}_{2}^{\mathrm{T}} \mathbf{A}^{\mathrm{T}} \mathbf{A} \mathbf{Q}_{2} = \mathbf{\Lambda} = \mathrm{diag}(\lambda_{1}, \lambda_{2}, \dots, \lambda_{n}).$$

Let $s_i = \sqrt{\lambda_i}$, then $s_i > 0$, i.e., $S = \text{diag}(s_1, s_2, ..., s_n)$ is positive definite, and $Q_2^T A^T A Q_2 = S^2$. Therefore,

$$S^{-1}Q_2^{\mathrm{T}}A^{\mathrm{T}}AQ_2S^{-1} = I, \tag{*}$$

which shows that $\mathbf{AQ}_{2}\mathbf{S}^{-1}$ is an orthogonal matrix, denoted by \mathbf{Q}_{1} .

Rewrite (*) and we can get $\mathbf{Q}_1^{\mathrm{T}} \mathbf{A} \mathbf{Q}_2 \mathbf{S}^{-1} = \mathbf{I}$, so $\mathbf{Q}_1^{\mathrm{T}} \mathbf{A} \mathbf{Q}_2 = \mathbf{S}$, or equivalently, $\mathbf{A} = \mathbf{Q}_1 \mathbf{S} \mathbf{Q}_2^{\mathrm{T}}$.

Theorem 2 (Singular Value Decomposition -- "SVD")

Any $m \times n$ real matrix with rank r can be factored into

$$A = U\Sigma V^{\mathrm{T}},$$

(real matrix) = (orthogonal) (rectangular diagonal) (orthogonal)

where U is orthogonal of degree m, V is orthogonal of degree n, and Σ is diagonal (but rectangular: $m \times n$).

Further, the columns of U are eigenvectors of AA^T , the columns of V are eigenvectors of A^TA , and the r positive entries $\sigma_1, \ldots, \sigma_r$ (called 'singular values') on the diagonal of Σ are the square roots of the nonzero eigenvalues of both AA^T and A^TA .

The factorization is called a **singular value decomposition** (奇异 值分解), or **SVD** for short.

$$A_{m \times n} = \mathbf{U}_{m \times m} \begin{bmatrix} \sigma_1 & & & & \\ & \sigma_2 & & \mathbf{0}_{r \times (n-r)} \\ & & \ddots & & \\ & & & \sigma_r & & \\ \hline & \mathbf{0}_{(m-r) \times r} & \mathbf{0}_{(m-r) \times (n-r)} \end{bmatrix}_{m \times n}^{T}$$

(orthogonal) (rectangular diagonal) (orthogonal) where $\sigma_1, \sigma_2, \dots, \sigma_r$ are the square roots of the nonzero eigenvalues of both AA^T and A^TA .

- U: the columns are orthonormal eigenvectors for AA^{T} .
- V: the columns are orthonormal eigenvectors for $A^{T}A$.

Remark 1 (other versions of SVD)

- For positive definite matrices A: Σ is Λ and $U\Sigma V^{\mathrm{T}}$ is identical to $Q\Lambda Q^{\mathrm{T}}$.
- For other symmetric matrices A, any negative eigenvalues in Λ become positive in Σ .
- For complex matrices A, Σ remains real but U and V become unitary (the complex version of orthogonal). We take $\underline{A} = U\Sigma V^{\mathrm{H}}$.

Remark 2
$$A = U\Sigma V^{T}$$
, so $A^{T} = V\Sigma^{T}U^{T}$, and hence
$$AA^{T} = (U\Sigma V^{T})(V\Sigma^{T}U^{T}) = U\Sigma\Sigma^{T}U^{T},$$
$$A^{T}A = (V\Sigma^{T}U^{T})(U\Sigma V^{T}) = V\Sigma^{T}\Sigma V^{T}.$$

U must be the eigenvector matrix for $\mathbf{A}\mathbf{A}^{\mathrm{T}}$. The eigenvalue matrix is $\mathbf{\Sigma}\mathbf{\Sigma}^{\mathrm{T}}$ (m by m) with $\sigma_1^2, \ldots, \sigma_r^2$ on the diagonal.

V must be the eigenvector matrix for $\mathbf{A}^{T}\mathbf{A}$. The eigenvalue matrix is $\mathbf{\Sigma}^{T}\mathbf{\Sigma}$ (n by n) with $\sigma_{1}^{2},...,\sigma_{r}^{2}$ on the diagonal.

Diagonal entries are eigenvalues for **AA**^T

Diagonal entries are eigenvalues for $A^T A$

Remark 3
$$AV = A[V_r : V_{n-r}] = [U_r : U_{m-r}] \begin{bmatrix} \Sigma_r & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{bmatrix} = U\Sigma.$$

where $A: m \times n$; $V: n \times n$; $V_r: n \times r$; $V_{n-r}: n \times (n-r)$; $U: m \times m$; $U_r: m \times r$; $U_{m-r}: m \times (m-r)$; $\Sigma_r: r \times r$; $\Sigma: m \times n$.

So
$$AV_r = U_r \Sigma_r$$
 and $AV_{n-r} = 0$.

Similarly, $\mathbf{A} = \mathbf{U} \mathbf{\Sigma} \mathbf{V}^{\mathrm{T}}$, so $\mathbf{A}^{\mathrm{T}} = \mathbf{V} \mathbf{\Sigma}^{\mathrm{T}} \mathbf{U}^{\mathrm{T}}$, and $\mathbf{A}^{\mathrm{T}} \mathbf{U} = \mathbf{V} \mathbf{\Sigma}^{\mathrm{T}}$, therefore

$$A^{\mathrm{T}}[U_r : U_{m-r}] = [V_r : V_{n-r}] \begin{bmatrix} \Sigma_r & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{bmatrix}.$$

So $\mathbf{A}^{\mathrm{T}}\mathbf{U}_{r} = \mathbf{V}_{r}\mathbf{\Sigma}_{r}$ and $\mathbf{A}^{\mathrm{T}}\mathbf{U}_{m-r} = \mathbf{0}$.

U and *V* give orthonormal bases for all four fundamental subspaces:

first r columns of U	column space of A
last $m-r$ columns of U	left nullspace of A
first r columns of V	row space of A
last $n-r$ columns of V	nullspace of A

Example 2 (SVD) Let
$$A = \begin{bmatrix} 1 & 2 \\ 0 & 0 \\ 0 & 0 \end{bmatrix}$$
.

Then
$$AA^{T} = \begin{bmatrix} 5 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}, A^{T}A = \begin{bmatrix} 1 & 2 \\ 2 & 4 \end{bmatrix}.$$

The nonzero eigenvalue of AA^{T} (and also $A^{T}A$) is 5, so the singular

value of
$$\boldsymbol{A}$$
 is $\sqrt{5}$, and $\boldsymbol{\Sigma} = \begin{bmatrix} \sqrt{5} & 0 \\ 0 & 0 \\ 0 & 0 \end{bmatrix}$.

Three unit eigenvectors of
$$\mathbf{A}\mathbf{A}^{\mathrm{T}}$$
 are $\begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}$, $\begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix}$. Thus $\mathbf{U} = \mathbf{I}$.

Finding two eigenvectors of
$$\mathbf{A}^{\mathrm{T}}\mathbf{A}$$
 gives rise to $\mathbf{V} = \begin{bmatrix} \frac{1}{\sqrt{5}} & -\frac{2}{\sqrt{5}} \\ \frac{2}{\sqrt{5}} & \frac{1}{\sqrt{5}} \end{bmatrix}$.

Therefore, the matrix A can be decomposed into

$$A = U\Sigma V^{\mathrm{T}}$$
.

It is easy to check that

$$\begin{bmatrix} 1 & 2 \\ 0 & 0 \\ 0 & 0 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} \sqrt{5} & 0 \\ 0 & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} \frac{1}{\sqrt{5}} & \frac{2}{\sqrt{5}} \\ -\frac{2}{\sqrt{5}} & \frac{1}{\sqrt{5}} \end{bmatrix}.$$

Any problem here? (see next slide)

Attention! The SVD chooses those bases in an extremely special way. They are more than just orthonormal. Actually,

$$Av_{j} = \sigma_{j}u_{j}, j = 1, ..., r.$$

Reason: Let v_j be a <u>unit</u> eigenvector of A^TA corresponding to the eigenvalue σ_j^2 (j = 1, ..., r), that is, $A^TAv_j = \sigma_j^2 v_j$. Thus

$$(AA^{\mathrm{T}})(Av_j) = AA^{\mathrm{T}}Av_j = A\sigma_j^2v_j = \sigma_j^2(Av_j),$$

namely, Av_j is an eigenvector of AA^T corresponding to the eigenvalue σ_j^2 .

The length of the vector $\mathbf{A}\mathbf{v}_j$ is σ_j because $\mathbf{v}_j^{\mathrm{T}}\mathbf{v}_j = 1$: $\|\mathbf{A}\mathbf{v}_i\|^2 = (\mathbf{A}\mathbf{v}_i)^{\mathrm{T}}(\mathbf{A}\mathbf{v}_i) = \mathbf{v}_i^{\mathrm{T}}\mathbf{A}^{\mathrm{T}}\mathbf{A}\mathbf{v}_i = \mathbf{v}_i^{\mathrm{T}}\sigma_i^2\mathbf{v}_i = \sigma_i^2\mathbf{v}_i^{\mathrm{T}}\mathbf{v}_i = \sigma_i^2.$

So the <u>unit</u> eigenvector $Av_j/\sigma_j = u_j$, and $Av_j = \sigma_j u_j$.

In other words, $AV = U\Sigma$.

How to construct the matrix V

 \mathbf{V} : the columns are orthonormal eigenvectors for $\mathbf{A}^{\mathrm{T}}\mathbf{A}$.

Let
$$v_1, v_2, \dots, v_n$$
 are columns of V , and let $V = \begin{bmatrix} v_1 & \cdots & v_r & v_{r+1} & \cdots & v_n \end{bmatrix} = \begin{bmatrix} V_r & \vdots & V_{n-r} \end{bmatrix}$

Then
$$A^{T}A = V(\Sigma^{T}\Sigma)V^{T}$$
 becomes

$$A^{\mathrm{T}}A\boldsymbol{v_1} = \sigma_1^2\boldsymbol{v_1}, \dots, A^{\mathrm{T}}A\boldsymbol{v_r} = \sigma_r^2\boldsymbol{v_r}, \ A^{\mathrm{T}}A\boldsymbol{v_{r+1}} = \boldsymbol{0}, \dots, A^{\mathrm{T}}A\boldsymbol{v_n} = \boldsymbol{0}$$

 v_1, \dots, v_r are eigenvectors of A^TA belonging to nonzero eigenvalues $\sigma_1^2, \dots, \sigma_r^2$ respectively.

 v_{r+1}, \dots, v_n are eigenvectors of $A^T A$ belonging to $\lambda = 0$.

How to construct the matrix U

$$A_{m \times n} = \mathbf{U}_{m \times m} \begin{bmatrix} \sigma_1 & & & & \\ & \sigma_2 & & \mathbf{0}_{r \times (n-r)} \\ & & \ddots & & \\ & & & \mathbf{0}_{(m-r) \times r} & \mathbf{0}_{(m-r) \times (n-r)} \end{bmatrix}_{m \times n}^{\mathsf{T}}$$

$$\Rightarrow A_{m \times n} V_{n \times n} = U_{m \times m} \Sigma_{m \times n}$$

$$A[v_1 \quad \cdots \quad v_r \quad v_{r+1} \quad \cdots \quad v_n] = [u_1 \quad \cdots \quad u_r \quad u_{r+1} \quad \cdots \quad u_m] \begin{bmatrix} \Sigma_r & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{bmatrix}$$

Comparing the first r columns of each side, we see that

$$A\mathbf{v}_{j} = \sigma_{j}\mathbf{u}_{j}, j = 1, \dots, r \Longrightarrow \mathbf{u}_{j} = \frac{1}{\sigma_{j}}A\mathbf{v}_{j}, j = 1, \dots, r$$

It follows from that each \mathbf{u}_j , $j=1,\dots,r$, is in the column space of A.

The dimension of the column space is r, so u_1, u_2, \dots, u_r form an orthonormal basis for C(A). The vector space $C(A)^{\perp} = N(A^T)$ has dimension m-r. u_{r+1}, \dots, u_m is an orthonormal basis for $N(A^T)$.

Singular Value Decomposition

Example 2' (SVD) Let
$$\mathbf{A} = \begin{bmatrix} 1 & 2 \\ 0 & 0 \\ 0 & 0 \end{bmatrix}$$
.

Then
$$AA^{T} = \begin{bmatrix} 5 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}, A^{T}A = \begin{bmatrix} 1 & 2 \\ 2 & 4 \end{bmatrix}.$$

The nonzero eigenvalue of AA^{T} (and also $A^{T}A$) is 5, so the singular value

of
$$\boldsymbol{A}$$
 is $\sigma_1 = \sqrt{5}$, and $\boldsymbol{\Sigma} = \begin{bmatrix} \sqrt{5} & 0 \\ 0 & 0 \\ 0 & 0 \end{bmatrix}$.

Two unit eigenvectors of
$$\mathbf{A}^{\mathrm{T}}\mathbf{A}$$
 are $\mathbf{v}_1 = \begin{bmatrix} \frac{1}{\sqrt{5}} \\ \frac{2}{\sqrt{5}} \end{bmatrix}$, $\mathbf{v}_2 = \begin{bmatrix} -\frac{2}{\sqrt{5}} \\ \frac{1}{\sqrt{5}} \end{bmatrix}$, corresponding

to the eigenvalues 5 and 0 respectively, so
$$V = \begin{bmatrix} \frac{1}{\sqrt{5}} & -\frac{2}{\sqrt{5}} \\ \frac{2}{\sqrt{5}} & \frac{1}{\sqrt{5}} \end{bmatrix}$$
.

By
$$\mathbf{A}\mathbf{v}_1/\sigma_1 = \mathbf{u}_1$$
, we get $\mathbf{u}_1 = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}$, and we choose $\mathbf{u}_2 = \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix}$, $\mathbf{u}_3 = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}$

to make **U** an orthogonal matrix.

Therefore, the matrix A can be decomposed into

$$A = U\Sigma V^{\mathrm{T}}$$
,

i.e.,
$$\begin{bmatrix} 1 & 2 \\ 0 & 0 \\ 0 & 0 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} \sqrt{5} & 0 \\ 0 & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} \frac{1}{\sqrt{5}} & \frac{2}{\sqrt{5}} \\ -\frac{2}{\sqrt{5}} & \frac{1}{\sqrt{5}} \end{bmatrix}.$$

Example 3 (SVD) Let
$$\mathbf{A} = \begin{bmatrix} -1 & 1 & 0 \\ 0 & -1 & 1 \end{bmatrix}$$
.

Then
$$AA^{T} = \begin{bmatrix} 2 & -1 \\ -1 & 2 \end{bmatrix}$$
, $A^{T}A = \begin{bmatrix} 1 & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 1 \end{bmatrix}$.

The eigenvalues of AA^{T} are 3 and 1, which are also the non-zero eigenvalues of $A^{T}A$. So $\sigma_{1} = \sqrt{3}$, $\sigma_{2} = 1$.

Finding three eigenvectors of $A^{T}A$ gives rise to

$$\mathbf{V} = \begin{bmatrix} \frac{1}{\sqrt{6}} & -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{3}} \\ -\frac{2}{\sqrt{6}} & 0 & \frac{1}{\sqrt{3}} \\ \frac{1}{\sqrt{6}} & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{3}} \end{bmatrix} = [\mathbf{v}_1 \quad \mathbf{v}_2 \quad \mathbf{v}_3].$$

Two unit eigenvectors of AA^{T} are

$$u_1 = \frac{Av_1}{\sigma_1} = \begin{bmatrix} -\frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{bmatrix}, \quad u_2 = \frac{Av_2}{\sigma_2} = \begin{bmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{bmatrix}.$$

Thus
$$\boldsymbol{U} = \begin{bmatrix} -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{bmatrix} = \frac{1}{\sqrt{2}} \begin{bmatrix} -1 & 1 \\ 1 & 1 \end{bmatrix}.$$

Now
$$\Sigma$$
 is a (2×3) -matrix $\Sigma = \begin{bmatrix} \sqrt{3} & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix}$, it is easy to get that

$$\mathbf{A} = \begin{bmatrix} -1 & 1 & 0 \\ 0 & -1 & 1 \end{bmatrix} = \mathbf{U} \mathbf{\Sigma} \mathbf{V}^{\mathrm{T}} = \frac{1}{\sqrt{2}} \begin{bmatrix} -1 & 1 \\ 1 & 1 \end{bmatrix} \begin{bmatrix} \sqrt{3} & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix} \begin{bmatrix} \frac{1}{\sqrt{6}} & -\frac{2}{\sqrt{6}} & \frac{1}{\sqrt{6}} \\ -\frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} \end{bmatrix}.$$

Example 4 Find the singular value decomposition(SVD) for

$$A = \begin{bmatrix} 1 & 1 \\ 1 & 1 \\ 0 & 0 \end{bmatrix}.$$

Solution.

$$A^{\mathrm{T}}A = \begin{bmatrix} 2 & 2 \\ 2 & 2 \end{bmatrix}$$

has eigenvalues 4 and 0, so the singular value of \mathbf{A} is $\sqrt{4} = 2$, and

$$\mathbf{\Sigma} = \begin{bmatrix} 2 & 0 \\ 0 & 0 \\ 0 & 0 \end{bmatrix}$$

Finding two eigenvectors corresponding to 4,0 of $A^{T}A$ gives rise to

$$V = \begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{-1}{\sqrt{2}} \end{bmatrix}.$$

Solution(continued).

$$\mathbf{u_1} = \frac{1}{\sigma_1} A \mathbf{v_1} = \frac{1}{2} \begin{bmatrix} 1 & 1 \\ 1 & 1 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \end{bmatrix} = \begin{bmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \\ 0 \end{bmatrix}$$

The remaining column vectors of U must form an orthonormal basis for $N(A^T)$, we can compute a basis for $N(A^T)$ in the usual way,

$$\boldsymbol{x}_2 = \begin{bmatrix} 1 \\ -1 \\ 0 \end{bmatrix}, \ \boldsymbol{x}_3 = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}.$$

Since these vectors are already orthogonal, it is not necessary to use the Gram–Schmidt process to obtain an orthonormal basis. We need only set

$$u_2 = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ -1 \\ 0 \end{bmatrix}, \quad u_3 = x_3 = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}.$$

Solution(continued).

It then follows that

$$A = \begin{bmatrix} 1 & 1 \\ 1 & 1 \\ 0 & 0 \end{bmatrix} = U\Sigma V^{\mathrm{T}}$$

$$= \begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} 2 & 0 \\ 0 & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \end{bmatrix}$$

Singular Value Decomposition Type The Factors Notes Form PA = LU**P**: permutation matrix The permutation matrix P is LUneeded when there are row factorization L: lower triangular matrix (A is any $m \times n$ exchanges during the row with unit diagonal (Gaussian matrix) reduction. (Otherwise, A = $U: m \times n$ echelon matrix elimination) LU) (When m = n, U is upper

triangular.) A = QR**Q**: matrix with orthonormal QR columns (When m = n, **Q**) factorization (A is any $m \times n$ becomes an orthogonal (Gram-Schmidt matrix with matrix.) orthogonalization) independent **R**: upper triangular and columns)

Singular Value

Decomposition

r)

(SVD)

When m = n, any invertible matrix can be factorized as a product of an orthogonal matrix and an upper triangular matrix. invertible $\bigcup \Phi : m \times m \text{ orthogonal}$ The columns of \boldsymbol{U} are $A = U\Sigma V^{\mathrm{T}}$ eigenvectors of AA^{T} , the matrix (A is any $m \times n$ columns of V are $\backslash / \mathbf{\hat{Q}} : n \times n \text{ orthogonal}$ matrix with rank eigenvectors of $A^{T}A$, and matrix the r positive entries on the is diagonal (but diagonal of Σ are the square rectangular: $\langle \! \rangle \times \langle \! \! \rangle \rangle$.

PA = LDU if U is upper

roots of the nonzero

and $A^{T}A$.

eigenvalues of both AA^{T}

triangular with unit diagonal.

III. Applications of SVD

There are lots of applications of SVD in various areas, including in communication of information and in mathematics.

Application I — polar decomposition / factorization (极分解)

Theorem 3 (*Polar factorization*) Every real <u>square matrix</u> can be factored into A = QS, where Q is <u>orthogonal</u> and S is <u>symmetric</u> <u>positive semidefinite</u>. If A is invertible then S is positive definite.

Proof. Let $A = U\Sigma V^{T}$ as above. Then

$$A = U\Sigma V^{\mathrm{T}} = (UV^{\mathrm{T}})(V\Sigma V^{\mathrm{T}})$$

Let
$$\mathbf{Q} = \mathbf{U}\mathbf{V}^{\mathrm{T}}$$
 and $\mathbf{S} = \mathbf{V}\mathbf{\Sigma}\mathbf{V}^{\mathrm{T}}$, $= (\bigvee \mathbf{\Sigma}^{\frac{1}{2}})(\mathbf{\Sigma}^{\frac{1}{2}})^{\mathsf{T}}$

then S is symmetric and positive semidefinite (because Σ is), and Q is an orthogonal matrix.

Example 5 Polar decomposition A = QS, where $A = \begin{bmatrix} 1 & -2 \\ 3 & -1 \end{bmatrix}$.

Solution
$$A = \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} 3 & -1 \\ -1 & 2 \end{bmatrix}$$
.

Remark 1 (Analogy) Every nonzero complex number z can be written as $z = re^{i\theta}$ (polar coordinates: 极坐标)

If we think of z as a 1 by 1 matrix, r corresponds to a positive definite matrix and $e^{i\theta}$ corresponds to an orthogonal matrix.

More exactly, since $\mathbf{e}^{i\theta}$ is complex and satisfies $\mathbf{e}^{-i\theta}\mathbf{e}^{i\theta}=1$, it forms a 1 by 1 unitary matrix: $\mathbf{U}^{\mathrm{H}}\mathbf{U}=\mathbf{I}$.

The SVD extends this "polar factorization" to matrices of any size.

Remark 2 A major use of the polar decomposition is in continuum mechanics (连续介质力学) and recently in robotics.

In any deformation, it is important to separate stretching from rotation, and that is exactly what QS achieves. (Q: a rotation, and possibly a reflection. The material feels no strain; S: has eigenvalues $\sigma_1, ..., \sigma_r$, which are the stretching factors (or compression factors).

https://www.geogebra.org/m/ts668wtf

Application II — the effective rank (有效秩)

The rank of a matrix: the number of independent rows (columns).

That can be hard to decide in computations!

- In exact arithmetic, counting the pivots is correct.
- Real arithmetic can be misleading—but discarding small pivots is not the answer.

For example, consider the following (ϵ is very small):

$$A = \begin{bmatrix} \epsilon & 2\epsilon \\ 1 & 2 \end{bmatrix}$$
 and $B = \begin{bmatrix} \epsilon & 1 \\ 0 & 0 \end{bmatrix}$ and $C = \begin{bmatrix} \epsilon & 1 \\ \epsilon & 1 + \epsilon \end{bmatrix}$

- (1) A has rank 1, although roundoff error will probably produce a second pivot. Both pivots will be small; how many do we ignore?
- (2) **B** has one small pivot, but we cannot pretend that its row is insignificant.
- (3) C has two pivots and its rank is 2, but its "effective rank" ought to be 1.

$$A = \begin{bmatrix} \epsilon & 2\epsilon \\ 1 & 2 \end{bmatrix}$$
 and $B = \begin{bmatrix} \epsilon & 1 \\ 0 & 0 \end{bmatrix}$ and $C = \begin{bmatrix} \epsilon & 1 \\ \epsilon & 1 + \epsilon \end{bmatrix}$

Solution (a more stable measure of rank):

Step 1 use A^TA or AA^T , which are symmetric but share the same rank as A.

Their eigenvalues—the singular values squared—are not misleading.

$$\mathbf{A}^{\mathrm{T}}\mathbf{A} = \begin{bmatrix} \epsilon^2 + 1 & 2\epsilon^2 + 2 \\ 2\epsilon^2 + 2 & 4\epsilon^2 + 4 \end{bmatrix}$$

<u>Step 2</u> Based on the accuracy of the data, we decide on a tolerance (like 10^{-6}) and count the singular values above it—that is the effective rank.

The examples above have effective rank 1 (when ϵ is very small).

Application III — image processing (图像处理)

$$A = U\Sigma V^{\mathrm{T}} = \begin{bmatrix} \mathbf{U}_r & \mathbf{U}_{m-r} \end{bmatrix} \begin{bmatrix} \mathbf{\Sigma}_r & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{bmatrix} \begin{bmatrix} \mathbf{V}_r^{\mathrm{T}} \\ \mathbf{V}_{n-r}^{\mathrm{T}} \end{bmatrix} = \mathbf{U}_r \mathbf{\Sigma}_r \mathbf{V}_r^{\mathrm{T}}.$$

where $A: m \times n$; $V: n \times n$; $V_r: n \times r$; $V_{n-r}: n \times (n-r)$; $U: m \times m$; $U_r: m \times r$; $U_{m-r}: m \times (m-r)$; $\Sigma_r: r \times r$; $\Sigma: m \times n$.

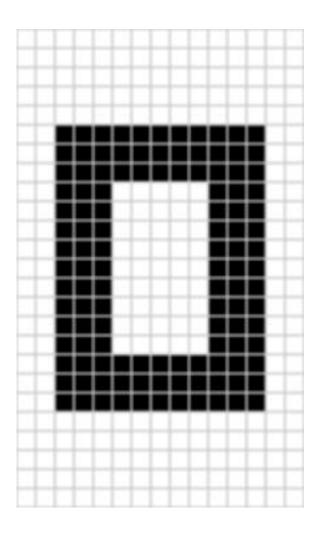
• Image compression (图像压缩)

例如一张 $m \times n$ 的图像,需要 $m \times n$ 的矩阵A来存储它.

而利用奇异值分解,则只需存储矩阵的奇异值(Σ_r 的对角线),奇异向量 U_r 和 V_r^{T} ,数目为 $r \times (m+n+1)$,而不再是 $m \times n$.

通常 $r \ll m$, n, 所以存储该图像所需的存储量减小了.

比值称 $\frac{m \times n}{r \times (m+n+1)}$ 为图像的压缩比, 其倒数称为<u>数据压缩率</u>.



 15×25 black or white pixels

	Г1	1	1	1	1	1	1	1	1	1	1	1	1	1	17
	1	1	1	1	1	1		1	1	1	1	1	1	1	1
	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
	1	1	1	1	1	1		1	1	1	1	1	1	1	1
	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
	1	1	0	0	0	0	0	0	0	0	0	0	0	1	1
	1	1	0	0	0	0	0	0	0	0	0	0	0	1	1
	1	1	0	0	0	0	0	0	0	0	0	0	0	1	1
	1	1	0	0	0	1	1	1	1	1	0	0	0	1	1
	1	1	0	0	0	1		1	1	1	0	0	0	1	1
	1	1	0	0	0	1	1	1	1	1	0	0	0	1	1
	1	1	0	0	0	1		1	1	1	0	0	0	1	1
M =	1	1	0	0	0	1	1	1	1	1	0	0	0	1	1
<i>IVI</i> —	1	1	0	0	0	1		1	1	1	0	0	0	1	1
	1	1	0	0	0	1	1	1	1	1	0	0	0	1	1
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	1	1	0	0	0	1	1	1	1	1	0	0	0	1	1
	1	1	0	0	0	0	0	0	0	0	0	0	0	1	1
	1	1	0	0	0	0	0	0	0	0	0	0	0	1	1
	1	1	0	0	0	0	0	0	0	0	0	0	0	1	1
	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
	1	1	1	1	1			1	1	1	1	1	1	1	1
	15500					1	1								10000
	L1	1	1	1	1	1	1	1	1	1	1	1	1	1	1]

0: black; 1: white pixel
The matrix *M* has 375 entries.

If we perform a singular value decomposition on M, we find there are only three non-zero singular values.

$$\sigma_1 = 14.72 , \sigma_2 = 5.22 , \sigma_3 = 3.31$$
 $\mathbf{M} = \mathbf{u}_1 \sigma_1 \mathbf{v}_1^{\mathrm{T}} + \mathbf{u}_2 \sigma_2 \mathbf{v}_2^{\mathrm{T}} + \mathbf{u}_3 \sigma_3 \mathbf{v}_3^{\mathrm{T}}$

This implies that we may represent the matrix using only 123 numbers rather than the 375 that appear in the matrix.

In this way, the singular value decomposition discovers the redundancy in the matrix and provides a format for eliminating it.



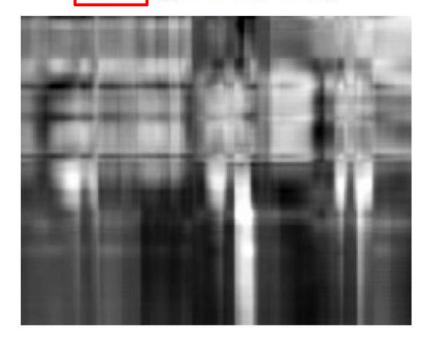
The organizing committee for the 1964 Gatlinburg/Householder meeting on *Numerical Algebra*. All six members of the committee – J. H. Wilkinson, Wallace Givens, George Forsythe, Alston Householder, Peter Henrici, and F. L. Bauer – have influenced MATLAB.

The following figure shows an image corresponding to a 176×260 matrix A and three images corresponding to lower rank approximations of A. The gentlemen in the picture are (from left to right) James H. Wilkinson, Wallace Givens, and George Forsythe (three pioneers in the field of numerical linear algebra).

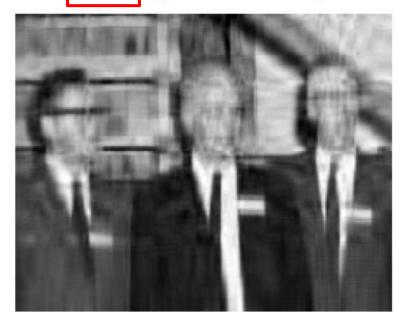
Original 176 by 260 Image



Rank 5 Approximation to Image



Rank 15 Approximation to Image



Rank 30 Approximation to Image



Courtesy Oakridge National Laboratory

The pictures are really striking, as more and more singular values are included.

At first you see nothing, and suddenly you recognize everything. The cost is in computing the SVD—this had become much more efficient, but it is expensive for a big matrix.

• Noise reduction (降噪)

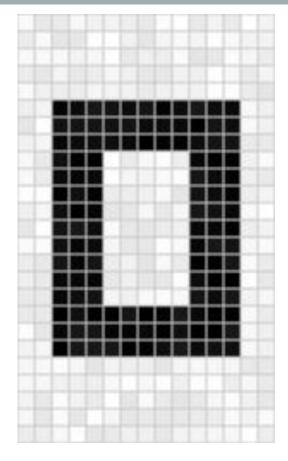
如果矩阵的奇异值从一个数开始 值远小于前面的奇异值,则可以 删去,这样在保证图像不失真的 前提下,进一步减小了存储量.

$$\sigma_1 = 14.15$$
 $\sigma_2 = 4.67$
 $\sigma_3 = 3.00$
 $\sigma_4 = 0.21$

$$\sigma_5 = 0.19$$

$$\sigma_{1.5} = 0.0$$

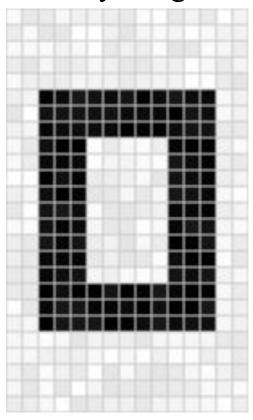
$$\sigma_{15}=0.05$$



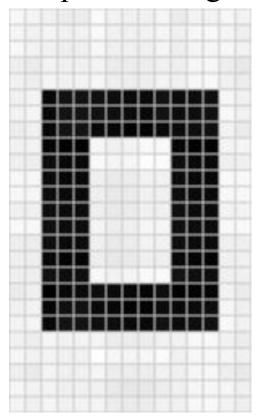
Clearly, the *first three singular values* are the most important, so we will assume that the others are due to the noise in the image and make the approximation:

$$\boldsymbol{M} \approx \boldsymbol{u}_1 \boldsymbol{\sigma}_1 \boldsymbol{v}_1^{\mathrm{T}} + \boldsymbol{u}_2 \boldsymbol{\sigma}_2 \boldsymbol{v}_2^{\mathrm{T}} + \boldsymbol{u}_3 \boldsymbol{\sigma}_3 \boldsymbol{v}_3^{\mathrm{T}}$$

Noisy image



Improved image



Application IV — least squares (最小二乘)

Recall that:

Theorem. If a system Ax = b is inconsistent (has no solution),

its least-squares solution minimizes $||Ax - b||^2$:

$$A^{\mathrm{T}}A\widehat{x} = A^{\mathrm{T}}b$$
 (Normal equations)

Moreover, if $\mathbf{A}^{\mathrm{T}}\mathbf{A}$ is invertible, then

$$\widehat{\boldsymbol{x}} = (\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A})^{-1}\boldsymbol{A}^{\mathrm{T}}\boldsymbol{b}.$$
 (Best estimate)

The projection of **b** onto the column space is the nearest point $A\hat{x}$:

$$p = A\widehat{x} = A(A^{T}A)^{-1}A^{T}b$$
. (Projection)

There is a simple way to decide whether $A^{T}A$ is invertible.

Theorem. The matrices $\mathbf{A}^{\mathrm{T}}\mathbf{A}$ and \mathbf{A} have the same nullspace.

In particular, if \mathbf{A} has full column rank, then $\mathbf{A}^{\mathrm{T}}\mathbf{A}$ is invertible.

Problem: If A has dependent columns then A^TA is not invertible and \hat{x} is not determined (not unique). Any vector in the nullspace could be added to \hat{x} .

We choose the solution: The optimal solution of Ax = b is the minimum length solution of $A^{T}A\hat{x} = A^{T}b$.

That minimum length solution will be called x^+ . It is our preferred choice as the best solution to Ax = b (which had no solution), and also to $A^T A \hat{x} = A^T b$ (which had too many).

We start with a diagonal example.

Example 6 *A* is diagonal, with dependent rows and dependent columns:

$$A\hat{x} = p$$
 is $\begin{bmatrix} \sigma_1 & 0 & 0 & 0 \\ 0 & \sigma_2 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} x_1 \\ \hat{x}_2 \\ \hat{x}_3 \\ \hat{x}_4 \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ 0 \end{bmatrix}$.

The columns all end with zero. In the column space, the closest vector to $\mathbf{b} = (b_1, b_2, b_3)^{\mathrm{T}}$ is $\mathbf{p} = (b_1, b_2, 0)^{\mathrm{T}}$.

The best we can do with Ax = b is to solve the first two equations, then $\hat{x}_1 = b_1/\sigma_1$ and $\hat{x}_2 = b_2/\sigma_2$.

Example 6 (Continued) To make \hat{x} as short as possible, we choose the totally arbitrary $\hat{x}_3 = \hat{x}_4 = 0$.

The minimum length solution is x^+ :

$$\boldsymbol{x}^{+} = \begin{bmatrix} b_{1}/\sigma_{1} \\ b_{2}/\sigma_{2} \\ 0 \\ 0 \end{bmatrix} = \begin{bmatrix} 1/\sigma_{1} & 0 & 0 \\ 0 & 1/\sigma_{2} & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} b_{1} \\ b_{2} \\ b_{3} \end{bmatrix}.$$

 $(A^+ \text{ is pseudoinverse of } A, \text{ and } x^+ = A^+ b \text{ is the shortest solution.})$

Remark. Based on this example, we know Σ^+ and x^+ for any rectangular diagonal matrix Σ :

$$\boldsymbol{\Sigma} = \begin{bmatrix} \sigma_{1} & & \\ & \ddots & \\ & & \sigma_{r} \end{bmatrix}, \quad \boldsymbol{\Sigma}^{+} = \begin{bmatrix} 1/\sigma_{1} & & \\ & \ddots & \\ & & 1/\sigma_{r} \end{bmatrix},$$

$$\boldsymbol{x}^{+} = \boldsymbol{\Sigma}^{+} \boldsymbol{b} = \begin{bmatrix} b_{1}/\sigma_{1} & & \\ \vdots & & \vdots \\ b_{r}/\sigma_{r} \end{bmatrix}, \quad and \ obviously \ \ \underline{(\boldsymbol{\Sigma}^{+})^{+} = \boldsymbol{\Sigma}}.$$

Now we look for x^+ in the general case.

We claim that: The shortest solution x^+ is always in the row space of A.

Remember that any vector \hat{x} can be split into a row space component x_r and a nullspace component: $\hat{x} = x_r + x_n$.

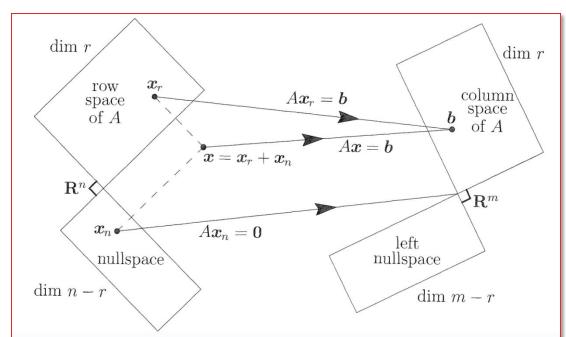
There are three important points about that splitting:

- 1. The row space component also solves $A^{T}Ax_{r} = A^{T}b$, because $Ax_n = 0.$
- 2. The components are orthogonal, and they obey Pythagoras's law:

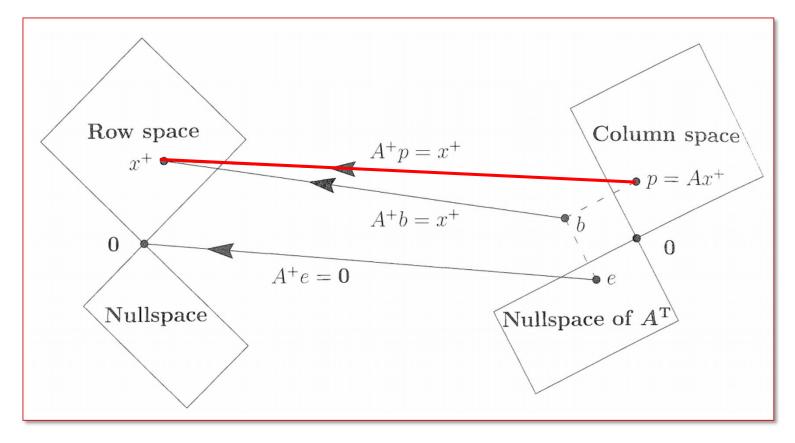
$$\|\widehat{\boldsymbol{x}}\|^2 = \|\boldsymbol{x}_r\|^2 + \|\boldsymbol{x}_n\|^2$$
, so $\widehat{\boldsymbol{x}}$ is shortest when $\boldsymbol{x}_n = \boldsymbol{0}$.

3. All solutions of $A^{T}A\widehat{x} = A^{T}b$

have the same x_r . That vector is x^+ .



All we are doing is to choose that vector, $x^+ = x_r$, as the best solution to Ax = b.



The pseudoinverse A^+ in the figure above starts with b and comes back to x^+ . It inverts A where A is invertible—between row space and column space. The pseudoinverse knocks out the left nullspace by sending it to zero, and it knocks out the nullspace by choosing x_r as x^+ .

Example 7 Ax = b is $-x_1 + 2x_2 + 2x_3 = 18$, with a whole plane of solutions.

According to our theory, the shortest solution should be in the row space of $A = \begin{bmatrix} -1 & 2 & 2 \end{bmatrix}$.

The multiple of that row that satisfies the equation is $x^+ = (-2,4,4)^T$.

The matrix that produces x^+ from b = [18] is the pseudoinverse A^+ . Whereas A was 1 by 3, this A^+ is 3 by 1:

$$A^{+} = [-1 \quad 2 \quad 2]^{+} = \begin{bmatrix} -\frac{1}{9} \\ \frac{2}{9} \\ \frac{2}{9} \end{bmatrix} \text{ and } A^{+}b = \begin{bmatrix} -\frac{1}{9} \\ \frac{2}{9} \\ \frac{2}{9} \end{bmatrix} [18] = \begin{bmatrix} -2 \\ 4 \\ 4 \end{bmatrix}.$$

The row space of \mathbf{A} is the column space of \mathbf{A}^+ .

Remark There are longer solutions like $(-2,5,3)^T$, $(-2,7,1)^T$, or $(-6,3,3)^T$, but they all have nonzero components from the nullspace.

Here is a formula for finding A^+ (next slide).

Theorem 4 If $A = U\Sigma V^T$ (the SVD), then its **pseudoinverse** is $A^+ = V\Sigma^+U^T$.

Remark

We can check this proposition in Example 7, where $A = [-1 \ 2 \ 2]$, and the singular value of A is $\sigma = 3$ — the square root of the eigenvalue of $AA^{T} = [9]$.

$$A = [-1 \ 2 \ 2] = U\Sigma V^{\mathrm{T}} = [1][3 \ 0 \ 0] \begin{bmatrix} -\frac{1}{3} & \frac{2}{3} & \frac{2}{3} \\ \frac{2}{3} & -\frac{1}{3} & \frac{2}{3} \\ \frac{2}{3} & \frac{2}{3} & -\frac{1}{3} \end{bmatrix},$$

and

$$\mathbf{V}\mathbf{\Sigma}^{+}\mathbf{U}^{\mathrm{T}} = \begin{bmatrix} -\frac{1}{3} & \frac{2}{3} & \frac{2}{3} \\ \frac{2}{3} & -\frac{1}{3} & \frac{2}{3} \\ \frac{2}{3} & \frac{2}{3} & -\frac{1}{3} \end{bmatrix} \begin{bmatrix} \frac{1}{3} \\ 0 \\ 0 \end{bmatrix} [1] = \begin{bmatrix} -\frac{1}{9} \\ \frac{2}{9} \\ \frac{2}{9} \end{bmatrix} = \mathbf{A}^{+}.$$

Theorem 4 If $A = U\Sigma V^{T}$ (the SVD), then its **pseudoinverse** is $A^{+} = V\Sigma^{+}U^{T}$

Proof Multiplication by the orthogonal matrix U^{T} leaves lengths unchanged:

$$||Ax - b|| = ||U\Sigma V^{\mathrm{T}}x - b|| = ||\Sigma V^{\mathrm{T}}x - U^{\mathrm{T}}b||.$$

Introduce the new unknown $y = V^{T}x = V^{-1}x$, which has the same length as x.

Then, minimizing ||Ax - b|| is the same as minimizing $||\Sigma y - U^{T}b||$.

Now Σ is diagonal and we know the best y^+ .

It is $y^+ = \Sigma^+ U^T b$, so the best x^+ is Vy^+ :

Shortest solution
$$x^+ = Vy^+ = V\Sigma^+U^Tb = A^+b$$
.

 Vy^+ is in the row space, and $A^TAx^+ = A^Tb$ from the SVD.

Key words:

Singular values
Singular Value Decomposition
Applications (I, II, III, IV)

Homework

See Blackboard

