**EXAMPLE 3** Orthogonally diagonalize the matrix $A = \begin{bmatrix} 3 & -2 & 4 \\ -2 & 6 & 2 \\ 4 & 2 & 3 \end{bmatrix}$, whose characteristic equation is

$$0 = -\lambda^3 + 12\lambda^2 - 21\lambda - 98 = -(\lambda - 7)^2(\lambda + 2)$$

Solution: The eigenvalues are then $\lambda_1 = 7$ with multiplicity 2 and $\lambda_2 = -2$ with multiplicity 1. Need to find the eigenvectors.

For $\lambda = 7$, need to solve the linear system

$$(A - 7I)\vec{x} = \begin{pmatrix} -4 & -2 & 4 \\ -2 & -1 & 2 \\ 4 & 2 & -4 \end{pmatrix}\begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = 0$$

It can be simplified to

$$2x_1 + x_2 - 2x_3 = 0$$

$$\Rightarrow \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} -\frac{x_2}{2} + x_3 \\ x_2 \\ x_3 \end{pmatrix} = x_2 \begin{pmatrix} -\frac{1}{2} \\ 1 \\ 0 \end{pmatrix} + x_3 \begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix}.$$

$$= \frac{x_2}{2} \underbrace{\begin{pmatrix} -1 \\ 2 \\ 0 \end{pmatrix}}_{\vec{x}_1} + x_3 \underbrace{\begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix}}_{\vec{x}_2}$$

The vectors $\vec{x}_1$, $\vec{x}_2$ are not orthonormal, we can follow Gram-Schmidt process to get an orthonormal basis of the eigenspace.

Let $\vec{v}_1 = x_1 = \begin{pmatrix} -1 \\ 2 \\ 0 \end{pmatrix}$, $\quad \vec{v}_2 = \vec{x}_2 - \dfrac{\langle x_2, \vec{v}_1 \rangle}{\langle \vec{v}_1, \vec{v}_1 \rangle} \vec{v}_1$

$$= \begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix} - \frac{-1}{5} \begin{pmatrix} -1 \\ 2 \\ 0 \end{pmatrix} = \frac{1}{5} \begin{pmatrix} 4 \\ 2 \\ 5 \end{pmatrix}.$$

Normalise them, get

$$\vec{u}_1 = \frac{\vec{v}_1}{\|\vec{v}_1\|} = \frac{1}{\sqrt{5}} \begin{pmatrix} -1 \\ 2 \\ 0 \end{pmatrix}, \quad \vec{u}_2 = \frac{\vec{v}_2}{\|\vec{v}_2\|} = \frac{1}{3\sqrt{5}} \begin{pmatrix} 4 \\ 2 \\ 5 \end{pmatrix}.$$

For $\lambda = -2$, solve the linear system

$$(A + 2I)\vec{x} = \begin{pmatrix} 5 & -2 & 4 \\ -2 & 8 & 2 \\ 4 & 2 & 5 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = 0$$

Solving it, get $\vec{x}_3 = \begin{pmatrix} -2 \\ -1 \\ 2 \end{pmatrix}$. Normalise it, get

$$\vec{u}_3 = \frac{1}{3} \begin{pmatrix} -2 \\ -1 \\ 2 \end{pmatrix}.$$

Then $\{\vec{u}_1, \vec{u}_2, \vec{u}_3\}$ form an orthonormal basis of $\mathbb{R}^3$, consisting of eigenvectors of $A$:

$$A[\vec{u}_1 \;\; \vec{u}_2 \;\; \vec{u}_3] = \underbrace{[\vec{u}_1 \;\; \vec{u}_2 \;\; \vec{u}_3]}_{P} \begin{bmatrix} 7 & & \\ & 7 & \\ & & -2 \end{bmatrix}$$

$$\Rightarrow \quad P^t A P = \begin{bmatrix} 7 & & \\ & 7 & \\ & & -2 \end{bmatrix} \quad \text{with} \quad P = \begin{pmatrix} -1/\sqrt{5} & 4/3\sqrt{5} & -2/3 \\ 2/\sqrt{5} & 2/3\sqrt{5} & -1/3 \\ 0 & 5/3\sqrt{5} & 2/3 \end{pmatrix}. \quad \boxtimes$$

# Applications to quadratic forms

- Recall that a quadratic form can be written as $Q(\mathbf{x}) = \mathbf{x}^t A\mathbf{x}$ for a symmetric matrix $A$, and that a change of variable $\mathbf{x} = P\mathbf{y}$ by an orthogonal matrix $P$ will change $Q$ to $Q(\mathbf{y}) = \mathbf{y}^t(P^tAP)\mathbf{y}$.
- Combined with the spectral theorem of symmetric matrices, we get the theorem

> **The Principal Axes Theorem**
>
> Let $A$ be an $n \times n$ symmetric matrix. Then there is an orthogonal change of variable, $\mathbf{x} = P\mathbf{y}$, that transforms the quadratic form $\mathbf{x}^T A\mathbf{x}$ into a quadratic form $\mathbf{y}^T D\mathbf{y}$ with no cross-product term.

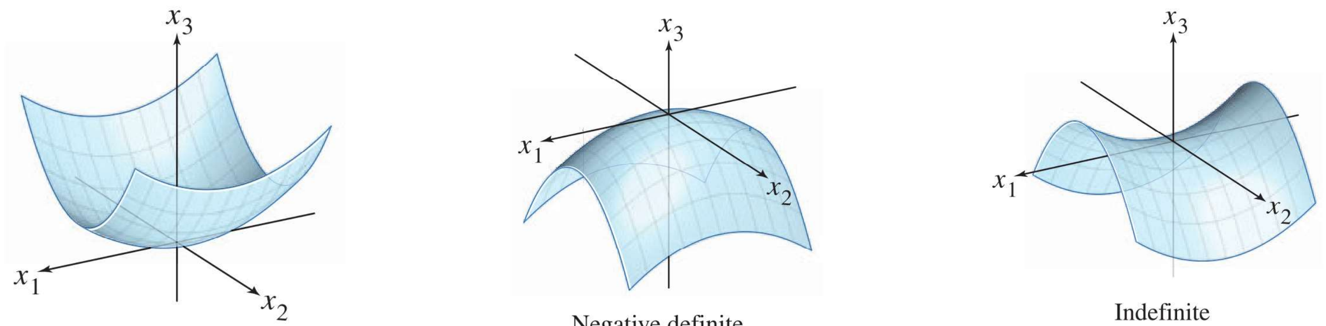
- The column vectors of $P$ are the eigenvectors of $A$, they are called the principle axes (主轴) of the quadratic form $Q$.

---

- In other words, with respect to the coordinate system given by the principal axes, the matrix for the quadratic form will be diagonal, i.e. it will be of the form $Q(\mathbf{y}) = \lambda_1 y_1^2 + \cdots + \lambda_n y_n^2$.
- Definition

> A quadratic form $Q$ is:
>
> a. **positive definite** if $Q(\mathbf{x}) > 0$ for all $\mathbf{x} \neq \mathbf{0}$,
>
> b. **negative definite** if $Q(\mathbf{x}) < 0$ for all $\mathbf{x} \neq \mathbf{0}$,
>
> c. **indefinite** if $Q(\mathbf{x})$ assumes both positive and negative values.

- It is called positive semi-definite (半正定) if $Q(\mathbf{x}) \geq 0$ for all $\mathbf{x}$, and negative semi-definite (半负定) if $Q(\mathbf{x}) \leq 0$ for all $\mathbf{x}$.



Positive definite

Negative definite

Indefinite

- Geometric meaning of the principle axes: Let

$$Q(x_1, x_2) = ax_1^2 + 2bx_1x_2 + cx_2^2 = \mathbf{x}^t \begin{bmatrix} a & b \\ b & c \end{bmatrix} \mathbf{x}$$

be a quadratic form in two variables, with $A = \begin{bmatrix} a & b \\ b & c \end{bmatrix}$ invertible. Consider the curve defined by the equation $Q(x_1, x_2) = r$ for some $r \neq 0$.

- In case that $A$ is diagonal, i.e. $Q(x_1, x_2) = ax_1^2 + cx_2^2$, the curve looks like:

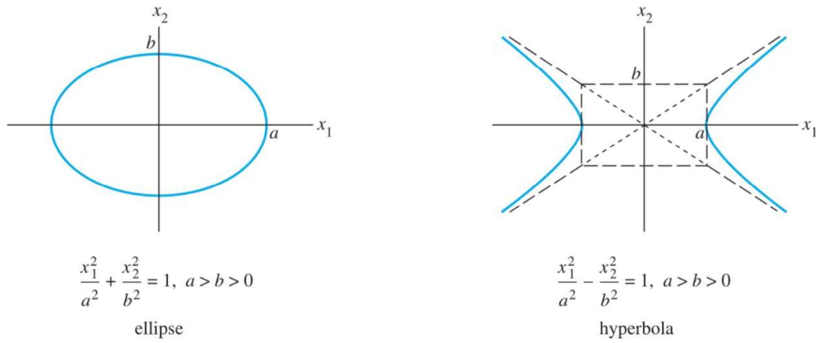



**FIGURE 2** An ellipse and a hyperbola in standard position.

- In general, the curve $Q(x_1, x_2) = r$ looks like

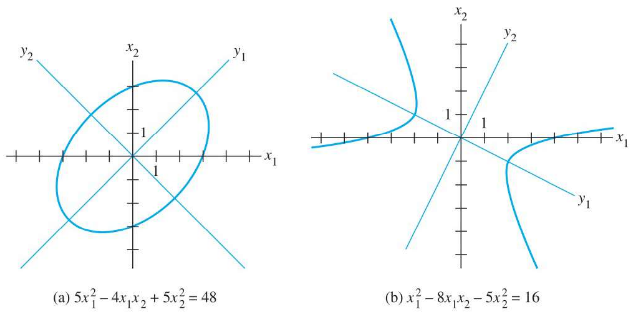



**FIGURE 3** An ellipse and a hyperbola *not* in standard position.

- The principle axes is the new coordinate system with respect to which the curve $Q(x_1, x_2) = r$ is in standard position.
- Observe that points on the $Q(x_1, x_2) = r$ such that $||\mathbf{x}||$ attains the maximum or minimum lie on the principal axes, and determines them uniquely.

- Theorem

**Quadratic Forms and Eigenvalues**

Let $A$ be an $n \times n$ symmetric matrix. Then a quadratic form $\mathbf{x}^T A \mathbf{x}$ is:

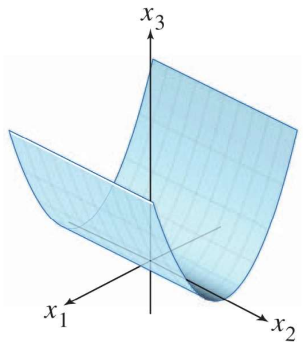
a. positive definite if and only if the eigenvalues of $A$ are all positive,

b. negative definite if and only if the eigenvalues of $A$ are all negative, or

c. indefinite if and only if $A$ has both positive and negative eigenvalues.

Proof: The change of variable $\vec{y} = P\vec{x}$ with $P$ orthogonal doesn't change whether $Q$ is positive definite, negative definite or indefinite. By the principle axe theorem, we can assume that $Q = \lambda_1 x_1^2 + \cdots + \lambda_n x_n^2$, $\lambda_1, \cdots, \lambda_n$ eigenvalues of $A$. The assertion is clear for such $Q$.

- A quadratic form is called degenerate, if the associated matrix has $0$ as one of its eigenvalues. With respect to the principal axis, it takes the form $Q(\mathbf{y}) = \lambda_1 y_1^2 + \cdots + \lambda_r y_r^2$, with $\lambda_1, \cdots, \lambda_r \neq 0$ and $r < n$. It is called non-degenerate otherwise.




(b) $z = 3x_1^2$

- Theorem: Let $A = \begin{bmatrix} a & b \\ b & a \end{bmatrix}$, the the quadratic form $Q(\mathbf{x}) = \mathbf{x}^t A \mathbf{x}$ is:

1. Positive definite if $a > 0$ and $\det(A) > 0$,
2. Negative definite if $a < 0$ and $\det(A) > 0$,
3. Indefinite if $\det(A) < 0$.
4. Degenerate if $\det(A) = 0$.

Proof By the previous theorem. it is enough to investigate the eigenvalues of A. Let $\lambda_1, \lambda_2$ be eigenvalues of A, then one can show $\lambda_1 + \lambda_2 = 2a$, $\lambda_1 \lambda_2 = \det(A)$ (why?). The assertion follows from analysis of $\lambda_1, \lambda_2$ with the two equalities $\boxtimes$

## Constraint optimization and Singular value decomposition

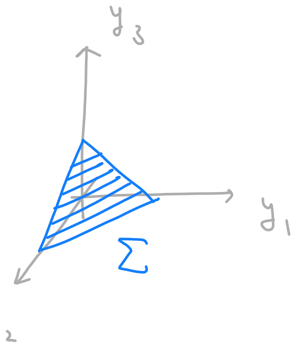
- Question: Let $Q(\mathbf{x}) = \mathbf{x}^t A \mathbf{x}$ be a quadratic form on $\mathbb{R}^n$, what is the maximum and minimum of $Q(\mathbf{x})$ for $||\mathbf{x}|| = 1$?

**EXAMPLE 1** Find the maximum and minimum values of $Q(\mathbf{x}) = 9x_1^2 + 4x_2^2 + 3x_3^2$ subject to the constraint $\mathbf{x}^T\mathbf{x} = 1$.

Solution: The constraint means that $x_1^2 + x_2^2 + x_3^2 = 1$.

Make a change of variable $y_i = x_i^2$, $i = 1, \cdots, 3$, the question can be reformulated as finding the maximum and minimum of $L(\vec{y}) = 9y_1 + 4y_2 + 3y_3$ under the constraint that $y_1 + y_2 + y_3 = 1$ and $y_1, y_2, y_3 \geq 0$.

As $L(\vec{y})$ and $y_1 + y_2 + y_3$ are both linear, the extremal values of $L(\vec{y})$ are attained at the vertices of $\Sigma$.




It is clear that

$$L(1,0,0) = 9 > L(0,1,0) = 4$$
$$> L(0,0,1) = 3$$

So $\operatorname{Max}\{ Q(\vec{x}) \mid \|x\| = 1 \} = Q(1,0,0) = 9$

$\operatorname{Min}\{ Q(\vec{x}) \mid \|x\| = 1 \} = Q(0,0,1) = 3$. $\boxed{5}$

- Let $m = \min\{Q(\mathbf{x}) \mid \|\mathbf{x}\| = 1\}$ and $M = \max\{Q(\mathbf{x}) \mid \|\mathbf{x}\| = 1\}$.
- Theorem

> Let $A$ be a symmetric matrix, and define $m$ and $M$ as in (2). Then $M$ is the greatest eigenvalue $\lambda_1$ of $A$ and $m$ is the least eigenvalue of $A$. The value of $\mathbf{x}^T A\mathbf{x}$ is $M$ when $\mathbf{x}$ is a unit eigenvector $\mathbf{u}_1$ corresponding to $M$. The value of $\mathbf{x}^T A\mathbf{x}$ is $m$ when $\mathbf{x}$ is a unit eigenvector corresponding to $m$.

Proof By the spectrum theorem of symmetric matrix, we can find an orthonormal basis $\vec{u}_1, \cdots, \vec{u}_n$ of $\mathbb{R}^n$, which are eigenvectors of $A$ with eigenvalues $\lambda_1 \geq \cdots \geq \lambda_n$.

Then with respect to the coordinate system $\vec{u}_1, \cdots, \vec{u}_n$, the quadratic form becomes

$$Q(\vec{y}) = (y_1\vec{u}_1 + \cdots + \vec{y}_n\vec{u}_n)^t A (y_1\vec{u}_1 + \cdots + y_n\vec{u}_n)$$

$$= (y_1\vec{u}_1 + \cdots + \vec{y}_n\vec{u}_n)^t \cdot (y_1 A\vec{u}_1 + \cdots + y_n A\vec{u}_n)$$

$$= (y_1\vec{u}_1 + \cdots + \vec{y}_n\vec{u}_n)^t \cdot (\lambda_1 y_1\vec{u}_1 + \cdots + \lambda_n \vec{y}_n\vec{u}_n)$$

$$= \sum_{i,j=1}^{n} (y_i\vec{u}_i)^t \cdot (\lambda_j y_j \vec{u}_j)$$

$$= \sum_{i,j=1}^{n} \lambda_j y_i y_j \underbrace{\vec{u}_i^t \cdot \vec{u}_j}_{\langle \vec{u}_i, \vec{u}_j \rangle = \begin{cases} 1 & \text{if } i=j \\ 0 & \text{otherwise} \end{cases}}$$

$$= \lambda_1 y_1^2 + \cdots + \lambda_n y_n^2.$$

Moreover, as $\vec{u}_1, \cdots, \vec{u}_n$ is orthonormal, we have

$$\| y_1\vec{u}_1 + \cdots + y_n\vec{u}_n \|^2 = y_1^2 + \cdots + y_n^2 \quad \text{(why?)}$$

So the question is reformulated as finding the extremal value of $Q(\vec{y}) = \lambda_1 y_1^2 + \cdots + \lambda_n y_n^2$ under the constraint that $y_1^2 + \cdots + y_n^2 = 1$. As before, let $z_i = y_i^2$, the question is reformulated as finding the extremal value of

$$L(\vec{z}) = \lambda_1 z_1 + \cdots + \lambda_n z_n \qquad \text{linear}$$

under the constraint that $z_1 + \cdots + z_n = 1$ and $z_1, \cdots, z_n \geq 0$.

linear

It is clear that $L(\vec{z})$ attains the maximal at $(1,0,\cdots,0)$ and the minimum at $(0,\cdots,0,1)$ as $\lambda_1 \geq \cdots \geq \lambda_n$.

Translated back to the quadratic form, get

$$\text{Max}\{Q(\vec{x}) \mid \|\vec{x}\|=1\} = \underbrace{Q(\vec{u}_1)}_{\text{correspond to } \vec{y}=(1,0,\cdots,0)} = \lambda_1$$

correspond to $\vec{y}=(1,0,\cdots,0)$.

$$\text{Min}\{Q(\vec{x}) \mid \|\vec{x}\|=1\} = Q(\vec{u}_n) = \lambda_n .$$

correspond to $\vec{y}=(0,\cdots,0,1)$.

$\boxed{S}$

- Theorem

Let $A$ be a symmetric $n \times n$ matrix with an orthogonal diagonalization $A = PDP^{-1}$, where the entries on the diagonal of $D$ are arranged so that $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$ and where the columns of $P$ are corresponding unit eigenvectors $\mathbf{u}_1, \ldots, \mathbf{u}_n$. Then for $k = 2, \ldots, n$, the maximum value of $\mathbf{x}^T A\mathbf{x}$ subject to the constraints

$$\mathbf{x}^T\mathbf{x} = 1, \quad \mathbf{x}^T\mathbf{u}_1 = 0, \quad \ldots, \quad \mathbf{x}^T\mathbf{u}_{k-1} = 0$$

is the eigenvalue $\lambda_k$, and this maximum is attained at $\mathbf{x} = \mathbf{u}_k$.

Proof The proof is exactly the same as before. The problem can be reformulated as looking for the extremal value of $\lambda_1 z_1 + \cdots + \lambda_n z_n$ under the constraint $z_1 + \cdots + z_n = 1$, $z_1, \cdots, z_n \geq 0$ and $\underset{x^t\vec{u}_1=0}{z_1} = \cdots = \underset{x^t\vec{u}_{k-1}=0}{z_{k-1}} = 0$, the result is then clear. $\boxed{S}$

- Question: Let $A$ be a $m \times n$ matrix, then $A$ defines the linear transformation $A : \mathbb{R}^n \to \mathbb{R}^m$, what is the maximum and minimum of $\|A\mathbf{x}\|$ for $\|\mathbf{x}\| = 1$?
- It is equivalent to ask for the maximum and minimum of $\|A\mathbf{x}\|^2 = \mathbf{x}^t A^t A\mathbf{x}$, which is a positive semi-definite quadratic form with matrix $A^t A$.
- Let $m = \min\{\|A\mathbf{x}\| \mid \|\mathbf{x}\| = 1\}$ and $M = \max\{\|A\mathbf{x}\| \mid \|\mathbf{x}\| = 1\}$.
- Theorem: Let $\mathbf{u}_1, \cdots, \mathbf{u_n}$ be an orthonormal basis of $\mathbb{R}^n$ consisting of eigenvalues of $A^t A$, such that the corresponding eigenvalues satisfies $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n \geq 0$. Then $M = \sqrt{\lambda_1} = \|A\mathbf{u}_1\|$ and $m = \sqrt{\lambda_n} = \|A\mathbf{u}_n\|$. Moreover, let $\lambda_1 \geq \cdots \geq \lambda_r$ be all the positive eigenvalues, then $A\mathbf{u_1}, \cdots, A\mathbf{u}_r$ forms an orthogonal basis of $\mathrm{Col}(A)$ and $A\mathbf{u}_{r+1} = \cdots = A\mathbf{u}_n = 0$.

Proof: Consider the quadratic form

$$Q(\vec{x}) = \|A\vec{x}\|^2 = \vec{x}^t A^t A \vec{x}.$$

Then with respect to the coordinate system $\{\vec{u}_1, \cdots, \vec{u}_n\}$, the quadratic form $Q(\vec{x})$ becomes

$$Q(\vec{y}) = \lambda_1 y_1^2 + \lambda_2 y_2^2 + \cdots + \lambda_n y_n^2.$$

It is then clear that

$$\|A\vec{u}_1\|^2 = Q\left(\begin{bmatrix}1\\0\\\vdots\\0\end{bmatrix}\right) = \max\{Q(\vec{y}) \mid \vec{y} \in \mathbb{R}^n\} = \lambda_1$$

$\vec{u}_1$ has coordinate $\begin{bmatrix}1\\0\\\vdots\\0\end{bmatrix}$ $\Rightarrow$ first assertion.

$$\|Au_n\|^2 = Q\left(\begin{bmatrix}0\\\vdots\\0\\1\end{bmatrix}\right) = \min\{Q(\vec{y}) \mid y \in \mathbb{R}^n\} = \lambda_n$$

$u_n$ has coordinate $\begin{bmatrix}0\\\vdots\\0\\1\end{bmatrix}$

For the second assertion, notice that

$$\langle A\vec{u}_i, A\vec{u}_j\rangle = (A\vec{u}_i)^t A\vec{u}_j = \vec{u}_i^{\,t} A^tA\vec{u}_j$$

$$= \langle \vec{u}_i, A^tA u_j\rangle = \langle \vec{u}_i, \lambda_j \vec{u}_j\rangle$$

$$= \lambda_j \langle \vec{u}_i, \vec{u}_j\rangle = \begin{cases} \lambda_j, & \text{if } i=j \\ 0, & \text{otherwise} \end{cases}$$

$\Rightarrow$ For $i=1,\cdots,r$, $\|A\vec{u}_i\|^2 = \lambda_i \neq 0$, so $A\vec{u}_i \neq 0$;

$i=r+1,\cdots,n$, $\|A\vec{u}_i\| = \lambda_i = 0$, so $A\vec{u}_i = 0$;

and $A\vec{u}_i$ is orthogonal to $A\vec{u}_j$ if $i\neq j$, $i,j=1,\cdots,r$.

$\Rightarrow$ $Col(A) = Im(A) = Span\{A\vec{u}_1,\cdots,A\vec{u}_r, \underset{0}{\underset{\shortparallel}{A\vec{u}_{r+1}}},\cdots,\underset{0}{\underset{\shortparallel}{A\vec{u}_n}}\}$

$= Span\{A\vec{u}_1,\cdots,A\vec{u}_r\}$

$\Rightarrow$ $A\vec{u}_1,\cdots,A\vec{u}_r$ is an orthogonal basis of $Col(A)$. $\boxed{\text{Q.E.D.}}$

- The theorem provides a very nice way to describe the linear transformation $A : \mathbb{R}^n \to \mathbb{R}^m$, this is the singular value decomposition of $A$.
- Definition: Let $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n \geq 0$ be the eigenvalues of $A^tA$, we call their square roots $\sqrt{\lambda_1} \geq \cdots \geq \sqrt{\lambda_n} \geq 0$ the singular values (奇异值) of $A$. It is clear that they are the length of the vectors $A\mathbf{u_1}, \cdots, A\mathbf{u}_n$.
- Notation: Let $\Sigma$ be the $m \times n$ matrix with non-zero entries only at the first $r$ diagonal positions and the diagonal terms being $\sqrt{\lambda_1} \geq \cdots \geq \sqrt{\lambda_r}$.

$$\Sigma = \left(\begin{array}{ccc|c} \sqrt{\lambda_1} & & & \\ & \ddots & & 0 \\ & & \sqrt{\lambda_r} & \\ \hline & 0 & & 0 \end{array}\right)_{m\times n}$$

- Singular value decomposition theorem: Let $\mathbf{u}_1, \cdots, \mathbf{u_n}$ be an orthonormal basis of $\mathbb{R}^n$ consisting of eigenvalues of $A^tA$, such that the corresponding eigenvalues satisfies $\lambda_1 \geq \cdots \geq \lambda_r > \lambda_{r+1} = \cdots = \lambda_n = 0$. Let $\mathbf{w}_i = A\mathbf{u}_i/\|A\mathbf{u}_i\|$ for $i = 1, \cdots, r$, and complete them with $w_{r+1}, \cdots, w_m$ such that they form an orthonormal basis of $\mathbb{R}^m$. Let $U = [\mathbf{u}_1 \ \cdots \ \mathbf{u}_n]$ and $W = [\mathbf{w}_1 \ \cdots \ \mathbf{w}_m]$, then $A = W\Sigma U^t$.

<u>proof</u> By the previous theorem, we have $A\vec{u}_1, \cdots, A\vec{u}_r$ forms an orthogonal basis of $\text{col}(A)$, and $\|A\vec{u}_i\| = \sqrt{\lambda_i}$, $i = 1, \cdots, r$, and $A\vec{u}_{r+1} = \cdots = A\vec{u}_n = 0$, so

$$A[\vec{u}_1 \ \cdots \ \vec{u}_r \ \vec{u}_{r+1} \cdots \ \vec{u}_n] = [A\vec{u}_1 \ \cdots \ A\vec{u}_r \ 0 \cdots 0]$$

$$= [\sqrt{\lambda_1}\,\vec{w}_1 \ \cdots \ \sqrt{\lambda_r}\,\vec{w}_r \ 0 \cdots 0]$$

$$= [\vec{w}_1 \ \cdots \ \vec{w}_r \ \vec{w}_{r+1} \cdots \ \vec{w}_m] \begin{bmatrix} \sqrt{\lambda_1} & & & & & \\ & \ddots & & & & \\ & & \sqrt{\lambda_r} & & & \\ & & & 0 & & \\ & & & & \ddots & \\ & & & & & 0 \end{bmatrix}_{m \times n}$$

$\Rightarrow AU = W\Sigma$, and so $A = W\Sigma U^{-1} = W\Sigma U^t$. $\blacksquare$