Definition 1 The singular values of an $m \times n$ matrix $A$ are the square roots of the eigenvalues of the symmetric $n \times n$ matrix $A^T A$ listed with their multiplicities in decreasing order

$$\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_n.$$  

Theorem 2 Let $L ( \vec{x} ) = A \vec{x}$ be a linear transformation from $\mathbb{R}^n$ to $\mathbb{R}^m$. Then there is an orthonormal basis $\vec{v}_1, \vec{v}_2, \ldots, \vec{v}_n$ of $\mathbb{R}^n$ such that

1. Vectors $L ( \vec{v}_1 ), \ldots, L ( \vec{v}_n )$ are orthogonal.
2. The lengths of vectors $L ( \vec{v}_1 ), \ldots, L ( \vec{v}_n )$ are the singular values $\sigma_1, \ldots, \sigma_n$ of matrix $A$.

Summary 3 (Singular-value Decomposition (SVD)) Let $A$ be a $m \times n$ matrix.

1. Find an orthonormal eigenbasis for matrix $A^T A$ (which is an $n \times n$ matrix). Write the eigenvectors as $\vec{v}_1, \vec{v}_2, \ldots, \vec{v}_n$ with the corresponding eigenvalues $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$.
2. Let $r = \text{rank}(A) \leq n$. We have $A \vec{v}_1, A \vec{v}_2, \ldots, A \vec{v}_r$ are orthogonal and nonzero with $\| A \vec{v}_i \| = \sigma_i$.
3. Write
   $\vec{u}_i = \frac{1}{\sigma_i} A \vec{v}_i$
   for $i = 1, 2, \ldots, r$.
4. If $r < m$, then pick an nonzero vector $\vec{w}$ which is outside the space span $\{ \vec{u}_1, \vec{u}_2, \ldots, \vec{u}_r \}$ (i.e. $\vec{w} \in \mathbb{R}^m$ but not a linear combination of $\vec{u}_1, \vec{u}_2, \ldots, \vec{u}_r$). Use Gram-Schmidt process to get an orthonormal basis of $\{ \vec{u}_1, \vec{u}_2, \ldots, \vec{u}_r, \vec{w} \}$. And then names $\vec{w}$ by $\vec{u}_{r+1}$.
5. Repeat Step 4 necessary times until you have an orthonormal basis of $\mathbb{R}^m$ which is $\{ \vec{u}_1, \vec{u}_2, \ldots, \vec{u}_r, \vec{u}_{r+1}, \ldots, \vec{u}_m \}$.
6. Write $V = [ \vec{v}_1, \vec{v}_2, \ldots, \vec{v}_n ]$.
7. Write $U = [ \vec{u}_1, \vec{u}_2, \ldots, \vec{u}_r, \vec{u}_{r+1}, \ldots, \vec{u}_m ]$.
8. Write $\Sigma = \begin{bmatrix} \sigma_1 & 0 & 0 & 0 \\ 0 & \ddots & 0 & 0 \\ 0 & 0 & \sigma_r & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}$ which is a $m \times n$ matrix.
9. Then we have the Singular-value Decomposition (SVD) $A = U \Sigma V^T$. 

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Example 4  Find an SVD for 
\[ \begin{bmatrix} 0 & 1 \\ 1 & 1 \\ 1 & 0 \end{bmatrix} \].

[Solution] Let us follow the above steps.

1. Consider 
\[ A^T A = \begin{bmatrix} 0 & 1 & 1 \\ 1 & 1 & 0 \end{bmatrix} \begin{bmatrix} 0 & 1 \\ 1 & 1 \\ 1 & 0 \end{bmatrix} = \begin{bmatrix} 2 & 1 \\ 1 & 2 \end{bmatrix}. \]

The characteristic equation is 
\[ 0 = \det (A^T A - \lambda I_2) = (2-\lambda)^2 - 1 = \lambda^2 - 4\lambda + 3. \]

We have two solutions for \( \lambda \), which are \( \lambda_1 = 3 \) and \( \lambda_2 = 1 \). And, the corresponding eigenvectors are \( \begin{bmatrix} 1 \\ 1 \end{bmatrix} \) and \( \begin{bmatrix} 1 \\ -1 \end{bmatrix} \), respectively. Moreover, we have an orthonormal eigenbasis of \( A^T A \) which is 
\[ \{ \begin{bmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{bmatrix}, \begin{bmatrix} \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} \end{bmatrix} \} \].

2. Let \( r = \text{rank}(A) = 2 \). We have
\[ A\tilde{v}_1 = \begin{bmatrix} \frac{1}{\sqrt{2}} \\ \frac{-1}{\sqrt{2}} \end{bmatrix} \]
with \( \sigma_1 = ||A\tilde{v}_1|| = \sqrt{3} \) and
\[ A\tilde{v}_1 = \begin{bmatrix} \frac{1}{\sqrt{2}} \\ 0 \\ \frac{1}{\sqrt{2}} \end{bmatrix} \]
with \( \sigma_2 = ||A\tilde{v}_2|| = 1 \).

3. Write
\[ \tilde{u}_1 = \frac{1}{\sigma_1} A\tilde{v}_1 = \frac{1}{\sqrt{3}} \begin{bmatrix} \frac{1}{\sqrt{2}} \\ \frac{-1}{\sqrt{2}} \end{bmatrix} = \begin{bmatrix} \frac{\sqrt{6}}{3} \\ \frac{-\sqrt{6}}{3} \end{bmatrix} \]
and
\[ \tilde{u}_2 = \frac{1}{\sigma_2} A\tilde{v}_2 = \frac{1}{1} \begin{bmatrix} \frac{-1}{\sqrt{2}} \\ 0 \\ \frac{1}{\sqrt{2}} \end{bmatrix} = \begin{bmatrix} \frac{-\sqrt{2}}{2} \\ 0 \\ \frac{\sqrt{2}}{2} \end{bmatrix} \].
4. Since $2 < 3$, we have to find $\vec{u}_3$ which is an unit vector perpendicular to $\vec{u}_1$ and $\vec{u}_2$, but not a linear combination of $\vec{u}_1$ and $\vec{u}_2$. Let $\vec{u}_3 = \vec{u}_1 \times \vec{u}_2 = \left( \begin{array}{c} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{3}} \\ \frac{1}{\sqrt{6}} \end{array} \right)$. We have

5. Now, $\{\vec{u}_1, \vec{u}_2, \vec{u}_3\}$ is an orthonormal basis of $\mathbb{R}^3$ already. So, we do not have to repeat Step 4

6. Write $V = [\vec{v}_1 \quad \vec{v}_2] = \left[ \frac{1}{\sqrt{2}} \quad \frac{1}{\sqrt{2}} \quad -\frac{1}{\sqrt{2}} \right]$.

7. Write $U = [\vec{u}_1 \quad \vec{u}_2 \quad \vec{u}_3] = \left[ \frac{1}{\sqrt{6}} \quad -\frac{1}{\sqrt{2}} \quad \frac{1}{\sqrt{3}} \right]$.

8. Write a $2 \times 3$ matrix $\Sigma = \left[ \begin{array}{ccc} \sqrt{3} & 0 \\ 0 & 1 \\ 0 & 0 \end{array} \right]$.

9. So the Singular-value Decomposition (SVD) is

$$A = U \Sigma V^T = \left[ \begin{array}{ccc} \frac{1}{\sqrt{6}} & -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{3}} \\ \frac{1}{\sqrt{6}} & \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{3}} \end{array} \right] \left[ \begin{array}{ccc} \sqrt{3} & 0 \\ 0 & 1 \\ 0 & 0 \end{array} \right] \left[ \begin{array}{ccc} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{6}} & -\frac{1}{\sqrt{3}} \end{array} \right].$$