

The Singular Value Decomposition: Introduction

L24

We finally come to the capstone of the class.

The SVD is a fundamental application of linear algebra for:

- Data Science
- Statistics (via PCA)
- Engineering
- etc.

Today we'll discuss the **outer product form** and the mechanics (plumbing?) of the SVD.

Theorem (SVD; outer product form):

(back to rectangular matrices)

Let A be an $m \times n$ matrix of rank r . Then

$$A = \sigma_1 u_1 v_1^T + \sigma_2 u_2 v_2^T + \cdots + \sigma_r u_r v_r^T$$

where:

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

$\{u_1, u_2, \dots, u_r\}$ is an orthonormal set in \mathbb{R}^m .

$\{v_1, v_2, \dots, v_r\}$ is an orthonormal set in \mathbb{R}^n .

What does this mean?

Idea: Think of the columns of A as data points.

Here's an informal description of what the SVD says.
Let's not worry about the σ 's or unit vectors yet.

$r=1$: If $u \in \mathbb{R}^n$, $v \in \mathbb{R}^n$ are nonzero vectors, then

$$uv^T = u(v_1 \cdots v_n) = \begin{pmatrix} | \\ v_1 u & \cdots & v_n u \\ | \end{pmatrix}$$

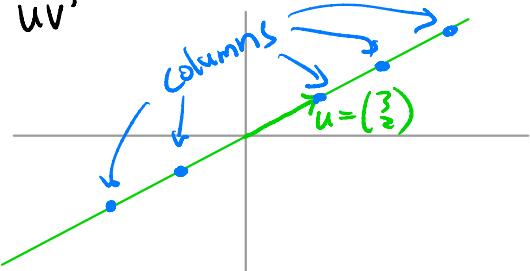
↑
weights ↓
multiples of u

This is an $m \times n$ matrix of **rank 1**, $\text{Col}(uv^T) = \text{Span}\{u\}$.

Let's plot the **columns** of uv^T (the data points).

$$\begin{pmatrix} 3 \\ 2 \end{pmatrix} \begin{pmatrix} -1 & 2 & 1 & 3 & -2 \end{pmatrix}$$

↑ ↓
 u v^T



The columns are $-1u, 2u, 1u, 3u, -2u$.

Upshot: A matrix A of rank 1 encodes data points (columns) that lie on a **line** ($\text{Col}(A)$). The outer product decomposition $A = uv^T$ tells you

which line: $\text{Span}\{u\}$

and which multiples of u : the entries of v^T .

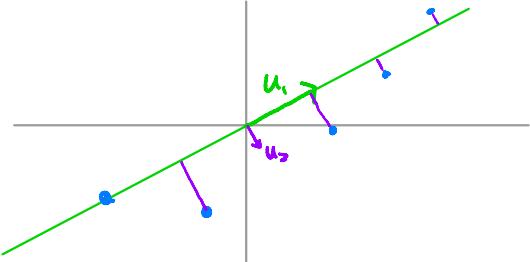
$r=2$: In this case, $A = u_1 v_1^T + u_2 v_2^T$.

$$\begin{aligned}
 u_1 v_1^T + u_2 v_2^T &= u_1(v_{11} \cdots v_{1n}) + u_2(v_{21} \cdots v_{2n}) \\
 &= \begin{pmatrix} & & & & \\ | & & & & | \\ v_{11}u_1 + v_{21}u_2 & \cdots & v_{1n}u_1 + v_{2n}u_2 & & \\ | & & & & | \\ & & & & \end{pmatrix} \\
 &\quad \text{linear combinations of } u_1, u_2
 \end{aligned}$$

This is an $m \times n$ matrix of rank 2: the columns are linear combinations of u_1, u_2 , so

$$\text{Col}(A) = \text{Span}\{u_1, u_2\} \text{ is a plane.}$$

Let's plot the columns of A (the data points).



$$A = \begin{pmatrix} u_1 \\ u_2 \end{pmatrix} \begin{pmatrix} v_1^T \\ v_2^T \end{pmatrix} = \begin{pmatrix} 3 \\ 2 \end{pmatrix} \begin{pmatrix} -1 & 2 & 1 & 3 & -2 \end{pmatrix} + \begin{pmatrix} -2 \\ -3 \end{pmatrix} \begin{pmatrix} 3 & 1 & 2 & -1 & 0 \end{pmatrix}$$

$v_1^T = \text{weights of } u_1$
 $v_2^T = \text{weights of } u_2$
 orthogonal

Upshot: A matrix A of rank 2 encodes data points (columns) that lie on a **plane** ($\text{Col}(A)$). The outer product decomposition $A = u_1 v_1^T + u_2 v_2^T$ tells you

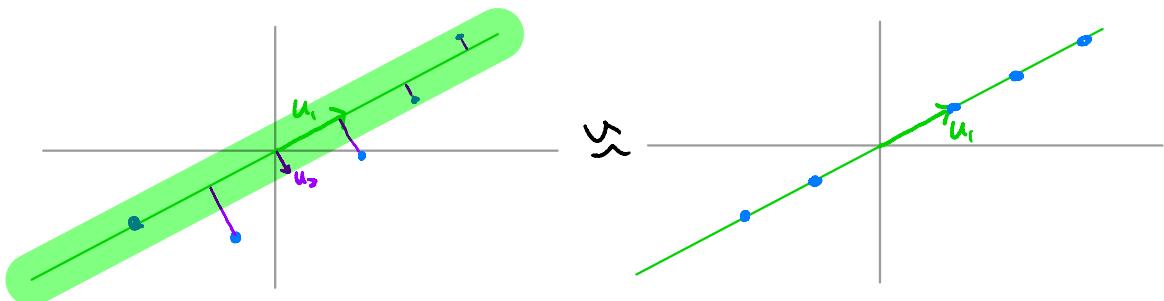
which plane: $\text{Span}\{u_1, u_2\}$

and the weights of u_1, u_2 : the entries of v_1^T, v_2^T .

BUT: $\left\| \begin{pmatrix} 3 \\ 2 \end{pmatrix} \right\| \gg \left\| \begin{pmatrix} -2 \\ 3 \end{pmatrix} \right\|$, so the $\begin{pmatrix} -2 \\ 3 \end{pmatrix}$ -direction is less important!

$$\begin{pmatrix} 3 \\ 2 \end{pmatrix} \begin{pmatrix} -1 & 2 & 1 & 3 & -2 \end{pmatrix} + \begin{pmatrix} -2 \\ 3 \end{pmatrix} \begin{pmatrix} 3 & 1 & 2 & -1 & 0 \end{pmatrix}$$

$$\approx \begin{pmatrix} 3 \\ 2 \end{pmatrix} \begin{pmatrix} -1 & 2 & 1 & 3 & -2 \end{pmatrix} \quad (\text{to one decimal place})$$



We've extracted important information:
our data points almost lie on a line!

In general, the SVD will find:

- the best-fit line
- the best-fit plane
- the best-fit 3-space

etc., for our data, all at once, and tell you how well they fit your data in the sense of orthogonal least squares. (L26, L27)

Why might you care?

- **Data compression:** if A is a 2×5 matrix and it almost has rank 1, then $A \approx U \mathbf{v}_1 \mathbf{v}_1^T$.
 $A = \begin{pmatrix} \bullet & \bullet & \bullet & \bullet & \bullet \\ \bullet & \bullet & \bullet & \bullet & \bullet \end{pmatrix}$ has 10 numbers, but $U \mathbf{v}_1 \mathbf{v}_1^T = \begin{pmatrix} \bullet \\ \bullet \end{pmatrix} (\bullet \bullet \bullet \bullet \bullet)$ only has 7.
- **Data analysis:** The SVD will reveal all approximate linear relations among your data points.
- **Dimension Reduction:** If our data points are in $\mathbb{R}^{1,000,000}$ but almost lie on a 100-dimensional subspace, then computers only need to use 100 numbers, not 1,000,000 (curse of dimensionality).
- **Statistics:** SVD finds important correlations. etc...

Mechanics of the SVD

Recall the statement of the

Theorem (SVD; outer product form):

Let A be an $m \times n$ matrix of rank r . Then

$$A = \sigma_1 u_1 v_1^T + \sigma_2 u_2 v_2^T + \cdots + \sigma_r u_r v_r^T$$

where:

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

- $\{u_1, u_2, \dots, u_r\}$ is an orthonormal set in \mathbb{R}^m .

- $\{v_1, v_2, \dots, v_r\}$ is an orthonormal set in \mathbb{R}^n .

The quantities in the theorem all have names.

Def:

- $\sigma_1, \sigma_2, \dots, \sigma_r$ are the **singular values**

- u_1, u_2, \dots, u_r are the **left singular vectors**

- v_1, v_2, \dots, v_r are the **right singular vectors**

} of A

Here are some formal consequences of the statement of the theorem.

Formal Consequence ①: For any vector $x \in \mathbb{R}^n$,

$$\begin{aligned}
 A_x &= (\sigma_1 u_1 v_1^T + \sigma_2 u_2 v_2^T + \cdots + \sigma_r u_r v_r^T) x \\
 &= \sigma_1 u_1 (v_1^T x) + \sigma_2 u_2 (v_2^T x) + \cdots + \sigma_r u_r (v_r^T x) \\
 &= \sigma_1 u_1 (v_1 \cdot x) + \sigma_2 u_2 (v_2 \cdot x) + \cdots + \sigma_r u_r (v_r \cdot x)
 \end{aligned}$$

$$\Rightarrow Ax = \alpha_1(v_1 \cdot x)u_1 + \alpha_2(v_2 \cdot x)u_2 + \dots + \alpha_r(v_r \cdot x)u_r$$

Formal Consequence 2: Taking $x = r_i$ above,

$$Ar_i = \sigma_1(v_i \cdot v_i)u_1 + \dots + \sigma_i(v_i \cdot v_i)u_i + \dots + \sigma_r(v_i \cdot v_i)u_r$$

$\uparrow 0 =$ $\uparrow 1$ $\uparrow 0$
 $\{v_1, v_2, \dots, v_r\}$ is orthonormal

Hence the singular vectors are related by:

$$A v_i = \sigma_i u_i \quad \xrightarrow{\text{If } u_i \neq 0} \quad \|A v_i\| = \sigma_i$$

Formal Consequence ③ :

$\{u_1, u_2, \dots, u_r\}$ is an orthonormal basis for $\text{Col}(A)$.

Indeed, ① shows that any $Ax \in \text{Span}\{u_1, u_2, \dots, u_r\}$, and ② shows $u_i = A\left(\frac{1}{\alpha_i}v_i\right) \in \text{Col}(A)$.

Formal Consequence ④: Take transposes:

$$\begin{aligned} A^T &= (\sigma_1 u_1 v_1^T + \sigma_2 u_2 v_2^T + \cdots + \sigma_r u_r v_r^T)^T \\ &= (\sigma_1 u_1 v_1^T)^T + (\sigma_2 u_2 v_2^T)^T + \cdots + (\sigma_r u_r v_r^T)^T \\ &= \sigma_1 v_1 u_1^T + \sigma_2 v_2 u_2^T + \cdots + \sigma_r v_r u_r^T \end{aligned}$$

This is also an SVD—the only difference is we switched the u_i 's and v_i 's.

The SVD of A^T is

$$A^T = \sigma_1 v_1 u_1^T + \sigma_2 v_2 u_2^T + \cdots + \sigma_r v_r u_r^T$$

In particular, A and A^T have the same:

- singular values $\sigma_1, \sigma_2, \dots, \sigma_n$, and
- singular vectors (switch right and left).

Since $\text{Col}(A^T) = \text{Row}(A)$, ③ + ④ imply:

Formal Consequence ⑤:

$\{v_1, v_2, \dots, v_r\}$ is an orthonormal basis for $\text{Row}(A)$.

Formal Consequence ⑥:

Applying ② and ④ gives

$$A^T u_i = \sigma_i v_i$$

and

$$\|A^T u_i\| = \sigma_i$$

Therefore,

$$A^T A v_i = A^T (\sigma_i u_i) = \sigma_i (A^T u_i) \stackrel{(above)}{=} \sigma_i (\sigma_i v_i) = \sigma_i^2 v_i$$

$$A A^T u_i = A (\sigma_i v_i) = \sigma_i (A v_i) \stackrel{(above)}{=} \sigma_i (\sigma_i u_i) = \sigma_i^2 u_i$$

$$A^T A v_i = \sigma_i^2 v_i$$

$$A A^T u_i = \sigma_i^2 u_i$$

This says:

v_1, v_2, \dots, v_r are **orthonormal eigenvectors**

of $A^T A$, with eigenvalues $\sigma_1^2, \sigma_2^2, \dots, \sigma_r^2$

u_1, u_2, \dots, u_r are **orthonormal eigenvectors**

of $A A^T$, with eigenvalues $\sigma_1^2, \sigma_2^2, \dots, \sigma_r^2$

This tells us how to prove the SVD exists / how to compute the SVD:

orthogonally diagonalize $S = A^T A$ or $A A^T$

Let's prove that the SVD exists.

Pay attention to **steps 1-2**: they illustrate the mechanics of the SVD.

Proof That the SVD Exists

Let $S = ATA$. Recall that S is positive-semidefinite, so its eigenvalues are ≥ 0 .

By the Spectral Theorem, $AM(\lambda) = GM(\lambda)$ for each eigenvalue λ , so I'll refer to both as the "multiplicity of λ ".

Let $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_n \geq 0$ be the eigenvalues of S , in decreasing order. If an eigenvalue has multiplicity d , it appears d times in this list.

Step 1: I claim that 0 is an eigenvalue of multiplicity $n-r$ ($r = \text{rank}(A)$).

(This just means 0 isn't an eigenvalue if $r=n$.)

Proof: The multiplicity of 0 is equal to

$$\begin{aligned} GM(0) &= \dim \text{Nul}(S - 0I_n) = \dim \text{Nul}(S) \\ &= \dim \text{Nul}(ATA). \end{aligned}$$

But $\text{Nul}(ATA) \stackrel{(L10)}{=} \text{Nul}(A)$ and $\dim \text{Nul}(A) \stackrel{(L8)}{=} n-r$, so the multiplicity of 0 is $n-r$. //

Step 1 implies $\lambda_{r+1} = \lambda_{r+2} = \dots = \lambda_n = 0$
 (zero is the smallest eigenvalue, so it comes last).

Therefore the nonzero eigenvalues of $S = A^T A$ are $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_r \geq 0$.

Now we can define the singular values and the singular vectors.

$$\sigma_1 = \sqrt{\lambda_1} \quad \sigma_2 = \sqrt{\lambda_2} \quad \dots \quad \sigma_r = \sqrt{\lambda_r}$$

Let $\{v_1, v_2, \dots, v_r\}$ be orthonormal eigenvectors of S with eigenvalues $\lambda_1, \lambda_2, \dots, \lambda_r$, respectively.

(This uses $AM = GM$ again: if λ_1 has multiplicity 2 then $\lambda_1 = \lambda_2$ and there are two LI λ_1 -eigenvectors.)

We know what the u 's have to be:

$$u_1 = \frac{1}{\sigma_1} A v_1 \quad u_2 = \frac{1}{\sigma_2} A v_2 \quad \dots \quad u_r = \frac{1}{\sigma_r} A v_r$$

Step 2: I claim $\{u_1, u_2, \dots, u_r\}$ is orthonormal.

Proof: $u_i \cdot u_j = \left(\frac{1}{\sigma_i} A v_i\right) \cdot \left(\frac{1}{\sigma_j} A v_j\right) = \left(\frac{1}{\sigma_i} A v_i\right)^T \left(\frac{1}{\sigma_j} A v_j\right)$

$$= \frac{1}{\sigma_i \sigma_j} (A v_i)^T (A v_j) = \frac{1}{\sigma_i \sigma_j} (v_i^T A^T)(A v_j)$$

$$\begin{aligned}
 &= \frac{1}{\sigma_i \sigma_j} v_i^T (A^T A) v_j = \frac{1}{\sigma_i \sigma_j} v_i^T S v_j \\
 &= \frac{1}{\sigma_i \sigma_j} v_i^T (\sigma_j^2 v_j) = \frac{\sigma_j}{\sigma_i} v_i^T v_j \\
 &= \frac{\sigma_j}{\sigma_i} v_i \cdot v_j
 \end{aligned}$$

Now we use the fact that $\{v_1, v_2, \dots, v_r\}$ is orthonormal:

$$i=j: \text{this} = \frac{\sigma_i}{\sigma_i} v_i \cdot v_i = 1$$

$$i \neq j: \text{this} = \frac{\sigma_i}{\sigma_i} v_i \cdot v_j = 0$$

//

Now we know what all of the singular values and vectors are supposed to be, so the only thing left to do is:

Step 3: Verification that

$$A = \sigma_1 u_1 v_1^T + \sigma_2 u_2 v_2^T + \dots + \sigma_r u_r v_r^T.$$

Proof: Let $B = \sigma_1 u_1 v_1^T + \sigma_2 u_2 v_2^T + \dots + \sigma_r u_r v_r^T$. We want to show that $A = B$. Recall (L11) that it's enough to show that $Ax = Bx$ for all vectors $x \in \mathbb{R}^n$.

Let $\{v_{r+1}, v_{r+2}, \dots, v_n\}$ be an orthonormal basis for the $(0\text{-eigenspace of } S) = \text{Nul}(S) = \text{Nul}(A)$.

Then $\{v_1, v_2, \dots, v_r, v_{r+1}, \dots, v_n\}$ is an orthonormal eigenbasis of S . (We just didn't do the 0 eigenvalue yet.)

(i) $Av_i = \alpha_i u_i = Bv_i$ ($i \leq r$):

$Av_i = \alpha_i u_i$ by definition of u_i .

$$\begin{aligned} Bv_i &= (\alpha_1 u_1 v_i^T + \alpha_2 u_2 v_2^T + \dots + \alpha_r u_r v_r^T) v_i \\ &= \alpha_1 (v_i \cdot v_i) u_1 + \dots + \alpha_r (v_i \cdot v_i) u_r + \dots + \alpha_n (v_i \cdot v_i) u_n \\ &= \alpha_i u_i, \text{ as in Formal Consequence 2} \end{aligned}$$

(ii) $Av_i = 0 = Bv_i$ ($i > r$):

$Av_i = 0$ because $v_i \in \text{Nul}(S) = \text{Nul}(A)$.

$$\begin{aligned} Bv_i &= (\alpha_1 u_1 v_i^T + \alpha_2 u_2 v_2^T + \dots + \alpha_r u_r v_r^T) v_i \\ &= \alpha_1 (v_i \cdot v_i) u_1 + \alpha_2 (v_i \cdot v_i) u_2 + \dots + \alpha_r (v_i \cdot v_i) u_r \\ &= 0 \text{ because } v_i \text{ is } \perp v_1, v_2, \dots, v_r \ (r \leq i). \end{aligned}$$

(iii) $Ax = Bx$ for any vector x :

Since $\{v_1, v_2, \dots, v_n\}$ is a basis for \mathbb{R}^n , we can expand in the eigenbasis:

$$x = x_1 v_1 + x_2 v_2 + \dots + x_n v_n$$

$$\Rightarrow Ax = A(x_1 v_1 + x_2 v_2 + \dots + x_n v_n)$$

$$= x_1 Av_1 + x_2 Av_2 + \dots + x_n Av_n$$

$$\stackrel{(i, ii)}{=} x_1 Bv_1 + x_2 Bv_2 + \dots + x_n Bv_n$$

$$= B(x_1 v_1 + x_2 v_2 + \dots + x_n v_n) = Bx //$$

Summary: Mechanics of the SVD

A : an $m \times n$ matrix of rank r

SVD:
$$A = \sigma_1 u_1 v_1^T + \sigma_2 u_2 v_2^T + \cdots + \sigma_r u_r v_r^T$$

$$Ax = \sigma_1(v_1 \cdot x)u_1 + \sigma_2(v_2 \cdot x)u_2 + \cdots + \sigma_r(v_r \cdot x)u_r$$

Singular Values: $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_r > 0$

$\sigma_1^2 \geq \sigma_2^2 \geq \cdots \geq \sigma_r^2$ are the nonzero eigenvalues of $A^T A$ and $A A^T$

Left singular Vectors: $\{u_1, u_2, \dots, u_r\}$

→ Orthonormal eigenvectors of $A A^T$:

$$A A^T u_i = \sigma_i^2 u_i$$

→ Orthonormal basis for $\text{Col}(A)$

Right singular Vectors: $\{v_1, v_2, \dots, v_r\}$

→ Orthonormal eigenvectors of $A^T A$:

$$A^T A v_i = \sigma_i^2 v_i$$

→ Orthonormal basis for $\text{Row}(A)$

The singular vectors are related by:

$$A v_i = \sigma_i u_i$$

$$A^T u_i = \sigma_i v_i$$

$$\|A v_i\| = \sigma_i = \|A u_i\|$$

SVD of A^T :
$$A^T = \sigma_1 v_1 u_1^T + \sigma_2 v_2 u_2^T + \cdots + \sigma_r v_r u_r^T$$

NB: ATA and AAT have the

some nonzero eigenvalues $\sigma_1^2, \sigma_2^2, \dots, \sigma_r^2$.

(We showed in Formal Consequence 6 that these are eigenvalues of ATA and AAT , and we showed in the proof that the other eigenvalues = 0.)

Q: What about the 0 eigenvalue?

Hint: What if A is a tall matrix with FCR?

The proof also gives a procedure to compute the SVD (see below).

NB: This is not the algorithm used in practice!

Efficiently computing the SVD is a hard problem.

See the course website for some links to real-world algorithms.

NB: If A is wide ($m < n$) then it's probably easier to compute the SVD of A^T :

ATA is $n \times n$ but AAT is $m \times m$, so it's easier to find eigenvalues and eigenvectors of AAT in this case.

Naive Schoolbook Procedure to Compute the SVD:

Let A be an $m \times n$ matrix of rank r .

(1) Compute the nonzero eigenvalues of $S = A^T A$:

$$\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_r > 0$$

(The λ_i 's appear multiple times if their multiplicities are ≥ 2 .)

→ There are automatically r of them (counted with multiplicity), and they are positive.

(2) Find an orthonormal basis for the λ_i -eigenspace ($i=1, 2, \dots, r$) → get an orthonormal set $\{v_1, v_2, \dots, v_r\}$ with $Sv_i = \lambda_i v_i$.

→ Since $AM(\lambda_i) = 0M(\lambda_i)$, you automatically get r vectors.

(3) Set $\sigma_i = \sqrt{\lambda_i}$ and $u_i = \frac{1}{\sigma_i} A v_i$ ($i=1, 2, \dots, r$).

Then $\{u_1, u_2, \dots, u_r\}$ is orthonormal, and

$$A = \sigma_1 u_1 v_1^T + \sigma_2 u_2 v_2^T + \dots + \sigma_r u_r v_r^T$$

is the SVD of A .

Eg: $A = \begin{pmatrix} 3 & 0 \\ 4 & 5 \end{pmatrix}$ $r=2$ (2 pivots / invertible)

(1) $S = A^T A = \begin{pmatrix} 25 & 20 \\ 20 & 25 \end{pmatrix}$

$$\begin{aligned} p(\lambda) &= \det(S - \lambda I_2) = \lambda^2 - 50\lambda + 225 \\ &= (\lambda - 45)(\lambda - 5) \end{aligned}$$

$$\text{so } \lambda_1 = 45 \geq \lambda_2 = 5$$

(2) Compute eigenspaces:

$$\lambda = 45 \quad \begin{pmatrix} -b \\ a-\lambda \end{pmatrix} = \begin{pmatrix} -20 \\ -20 \end{pmatrix} \rightsquigarrow v_1 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

$$\lambda = 5 \quad \begin{pmatrix} -b \\ a-\lambda \end{pmatrix} = \begin{pmatrix} -20 \\ 20 \end{pmatrix} \rightsquigarrow v_2 = \frac{1}{\sqrt{10}} \begin{pmatrix} -1 \\ 1 \end{pmatrix}$$

(3) $\sigma_1 = \sqrt{\lambda_1} = 3\sqrt{5} \quad \sigma_2 = \sqrt{\lambda_2} = \sqrt{5}$

$$u_1 = \frac{1}{\sigma_1} A v_1 = \frac{1}{3\sqrt{5}} \begin{pmatrix} 3 & 0 \\ 4 & 5 \end{pmatrix} \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix} = \frac{1}{3\sqrt{10}} \begin{pmatrix} 3 \\ 9 \end{pmatrix} = \frac{1}{\sqrt{10}} \begin{pmatrix} 1 \\ 3 \end{pmatrix}$$

$$u_2 = \frac{1}{\sigma_2} A v_2 = \frac{1}{\sqrt{5}} \begin{pmatrix} 3 & 0 \\ 4 & 5 \end{pmatrix} \frac{1}{\sqrt{2}} \begin{pmatrix} -1 \\ 1 \end{pmatrix} = \frac{1}{\sqrt{10}} \begin{pmatrix} -3 \\ 1 \end{pmatrix}$$

Check: $\|u_1\| = \frac{1}{\sqrt{10}} \sqrt{1^2 + 3^2} = 1 \quad u_1 \cdot u_2 = 0$

$$\|u_2\| = \frac{1}{\sqrt{10}} \sqrt{(-3)^2 + 1^2} = 1$$



SVR:

$$\begin{pmatrix} 3 & 0 \\ 4 & 5 \end{pmatrix} = 3\sqrt{5} \cdot \frac{1}{\sqrt{10}} \begin{pmatrix} 1 \\ 3 \end{pmatrix} \cdot \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \end{pmatrix} + \sqrt{5} \cdot \frac{1}{\sqrt{10}} \begin{pmatrix} -3 \\ 1 \end{pmatrix} \cdot \frac{1}{\sqrt{2}} \begin{pmatrix} -1 & 1 \end{pmatrix}$$

NB: You don't want to cancel the $\sqrt{5}$'s and $\sqrt{10}$'s here!

You want to remember that $\sigma_1 = 3\sqrt{5}$ & $\sigma_2 = \sqrt{5}$.