Singular Value Decomposition

An Example

Calculating a singular value decomposition

Consider the following matrix:
(Lay 7.4, Example 3)

```
Clear[a, aTax, evals, evecs, Λ, V, v1, v2, v3, Σ, σ1, σ2, U, u1, u2]
```

$$a = \begin{pmatrix} 4 & 11 & 14 \\ 8 & 7 & -2 \end{pmatrix};$$

■ Find the eigendata for $A^T A$.

```
aTa = Transpose[a].a;

evals = Eigenvalues[aTa];
Λ = DiagonalMatrix[evals];
% // MatrixForm
```

$$\begin{pmatrix} 360 & 0 & 0 \\ 0 & 90 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

```
evecs = Eigenvectors[aTa];
% // MatrixForm
```

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

■ Construct V.

The columns of the matrix V are the orthonormal eigenvectors of $A^T A$, taken in the proper order.

```
v1 = evecs[[1]] / Norm[evecs[[1]]];
v2 = evecs[[2]] / Norm[evecs[[2]]];
v3 = evecs[[3]] / Norm[evecs[[3]]];

V = Transpose[{v1, v2, v3}];
% // MatrixForm
```

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

Check that the columns of V are orthonormal.

```
Transpose[V].V;
% // MatrixForm
```

$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

Check the diagonalization.

```
aTa == V.Λ.Inverse[V]

True
```

■ Construct Σ .

```
<< LinearAlgebra`MatrixManipulation`
```

```
singularValues = {σ1, σ2, σ3} = √evals

Σ = ZeroMatrix[2, 3];
Σ[[1, 1]] = σ1;
Σ[[2, 2]] = σ2;
Σ // MatrixForm
```

$\{6\sqrt{10}, 3\sqrt{10}, 0\}$

$$\begin{pmatrix} 6\sqrt{10} & 0 & 0 \\ 0 & 3\sqrt{10} & 0 \end{pmatrix}$$

Construct U .

A has rank 2. The two columns of U are the normalized vectors A.v1 and A.v2.

```
u1 = (1 / σ1) a.v1;
u2 = (1 / σ2) a.v2;

U = Transpose[{u1, u2}];
% // MatrixForm
```

$$\begin{pmatrix} \frac{3}{\sqrt{10}} & \frac{1}{\sqrt{10}} \\ \frac{1}{\sqrt{10}} & -\frac{3}{\sqrt{10}} \end{pmatrix}$$

Check the singular value decomposition, A == U.Σ.V^T.

```
Print[a // MatrixForm, "==", U // MatrixForm,
  ".", Σ // MatrixForm, ".", Transpose[V] // MatrixForm];

a == U.Σ.Transpose[V]
```

$$\begin{pmatrix} 4 & 11 & 14 \\ 8 & 7 & -2 \end{pmatrix} == \begin{pmatrix} \frac{3}{\sqrt{10}} & \frac{1}{\sqrt{10}} \\ \frac{1}{\sqrt{10}} & -\frac{3}{\sqrt{10}} \end{pmatrix} . \begin{pmatrix} 6\sqrt{10} & 0 & 0 \\ 0 & 3\sqrt{10} & 0 \end{pmatrix} . \begin{pmatrix} \frac{1}{3} & \frac{2}{3} & \frac{2}{3} \\ -\frac{2}{3} & -\frac{1}{3} & \frac{2}{3} \\ \frac{2}{3} & -\frac{2}{3} & \frac{1}{3} \end{pmatrix}$$

True

Compare with *Mathematica*'s singular value decomposition.

Mathematica's numerical result.

```
a = (4.  11  14
     8   7   -2);
{u, w, v} = SingularValueDecomposition[a];

Print[a // MatrixForm, "==", u // MatrixForm,
  ".", w // MatrixForm, ".", Transpose[v] // MatrixForm];
a == u.w.Transpose[v]
```

```
(4.  11  14)    (-0.948683   0.316228)
(8   7   -2) == (-0.316228  -0.948683) .

                                  (-0.333333  -0.666667  -0.666667)
 (18.9737  0.       0.)           (-0.666667  -0.333333   0.666667)
 (0.       9.48683  0.)  .        (-0.666667   0.666667  -0.333333)
```

```
True
```

Our numerical result.
These two results agree up to a sign change on some rows and columns.

```
Print[a // MatrixForm, "==", U // MatrixForm // N, ".",
  Σ // MatrixForm // N, ".", Transpose[V] // MatrixForm // N];

a == U.Σ.Transpose[V]
```

```
(4.  11  14)    (0.948683   0.316228)
(8   7   -2) == (0.316228  -0.948683) .

                                  ( 0.333333   0.666667   0.666667)
 (18.9737  0.       0.)           (-0.666667  -0.333333   0.666667)
 (0.       9.48683  0.)  .        ( 0.666667  -0.666667   0.333333)
```

```
True
```

The Four Fundamental Subspaces

Consider the matrix of the previous example, ...

```
a = (4  11  14
     8   7  -2);
```

... and its singular value decomposition, A == U.Σ.V^T.

```
Print[a // MatrixForm, "==", U // MatrixForm,
  ".", Σ // MatrixForm, ".", Transpose[V] // MatrixForm];

a == U.Σ.Transpose[V]
```

$$\begin{pmatrix} 4 & 11 & 14 \\ 8 & 7 & -2 \end{pmatrix} == \begin{pmatrix} \frac{3}{\sqrt{10}} & \frac{1}{\sqrt{10}} \\ \frac{1}{\sqrt{10}} & -\frac{3}{\sqrt{10}} \end{pmatrix} . \begin{pmatrix} 6\sqrt{10} & 0 & 0 \\ 0 & 3\sqrt{10} & 0 \end{pmatrix} . \begin{pmatrix} \frac{1}{3} & \frac{2}{3} & \frac{2}{3} \\ -\frac{2}{3} & -\frac{1}{3} & \frac{2}{3} \\ \frac{2}{3} & -\frac{2}{3} & \frac{1}{3} \end{pmatrix}$$

```
True
```

a is an mxn matrix with rank r.

```
m = 2;
n = 3;
r = 2;
```

The **singular value decomposition** of a displays **orthogonal bases** for the **four fundamental subspaces** of a as follows:
(See Lay 7.4, p479)

```
(* α == [v1,v2] == [v₁,...,vᵣ]   == basis for Row a *)
(* β == [v3]    == [vᵣ₊₁,...,vₙ] == basis for Nul a *)

(* γ == [u1,u2] == [u₁,...,uᵣ]   == basis for Row aᵀ == Col a *)
(* δ == []      == [uᵣ₊₁,...,uₘ] == basis for Nul aᵀ *)
```

The Moore-Penrose Inverse and Least-Squares Solutions

Consider the matrix of the previous example, ...

$$a = \begin{pmatrix} 4 & 11 & 14 \\ 8 & 7 & -2 \end{pmatrix};$$

... and its singular value decomposition, A == U.Σ.V^T .

```
Print[a // MatrixForm, "==", U // MatrixForm,
  ".", Σ // MatrixForm, ".", Transpose[V] // MatrixForm];

a == U.Σ.Transpose[V]
```

$$\begin{pmatrix} 4 & 11 & 14 \\ 8 & 7 & -2 \end{pmatrix} == \begin{pmatrix} \frac{3}{\sqrt{10}} & \frac{1}{\sqrt{10}} \\ \frac{1}{\sqrt{10}} & -\frac{3}{\sqrt{10}} \end{pmatrix} . \begin{pmatrix} 6\sqrt{10} & 0 & 0 \\ 0 & 3\sqrt{10} & 0 \end{pmatrix} . \begin{pmatrix} \frac{1}{3} & \frac{2}{3} & \frac{2}{3} \\ -\frac{2}{3} & -\frac{1}{3} & \frac{2}{3} \\ \frac{2}{3} & -\frac{2}{3} & \frac{1}{3} \end{pmatrix}$$

```
True
```

a is an mxn matrix with rank r.

```
m = 2;
n = 3;
r = 2;
```

The **Moore-Penrose Inverse, A+,** or **pseudoinverse** of A is computed from its singular value decomposition, A == U.Σ.V^T, as follows:
(See Lay 7.4, p479)

```
Ur = U[[All, {1, 2}]];
Dr = DiagonalMatrix[{σ1, σ2}];
Vr = V[[All, {1, 2}]];

aPlus = Vr.Inverse[Dr].Transpose[Ur];

Print[aPlus // MatrixForm, " == ", Vr // MatrixForm, ".",
  Inverse[Dr] // MatrixForm, ".", Transpose[Ur] // MatrixForm];
```

$$\begin{pmatrix} -\frac{1}{180} & \frac{13}{180} \\ \frac{1}{45} & \frac{2}{45} \\ \frac{1}{18} & -\frac{1}{18} \end{pmatrix} == \begin{pmatrix} \frac{1}{3} & -\frac{2}{3} \\ \frac{2}{3} & -\frac{1}{3} \\ \frac{2}{3} & \frac{2}{3} \end{pmatrix} . \begin{pmatrix} \frac{1}{6\sqrt{10}} & 0 \\ 0 & \frac{1}{3\sqrt{10}} \end{pmatrix} . \begin{pmatrix} \frac{3}{\sqrt{10}} & \frac{1}{\sqrt{10}} \\ \frac{1}{\sqrt{10}} & -\frac{3}{\sqrt{10}} \end{pmatrix}$$

Suppose we wish to solve the least-squares problem A.x == b.

```
(* a.x == b *)
```

Let

```
(* xHat = aPlus.b *)
```

Then,

```
(* a.xHat == (Ur.D.Vr^T).(Vr.D^-1.Ur^T.b) ==
  (Ur.D.D^-1.Ur^T.b) == Ur.Ur^T.b == bHat *)
```

where bHat is the orthogonal projection of b onto Col A == Col Ur.
Therefore, **xHat is a least squares solution of A.x == b**.

It can be shown that this xHat, obtained via the Moore-Penrose inverse of A,
is the **shortest least-squares solution** of A.x == b
(See Lay 7.4, p480)

Another Example

Calculating another singular value decomposition

Consider the following matrix:
(Lay 7.4, Example 4)

```
Clear[a, aTax, evals, evecs, Λ, V, v1, v2, v3, Σ, σ1, σ2, U, u1, u2]

a = ( 1  -1
     -2   2
      2  -2 );
```

Find the eigendata for $A^T A$.

```
aTa = Transpose[a].a;

evals = Eigenvalues[aTa];
Λ = DiagonalMatrix[evals];
% // MatrixForm

( 18  0
  0   0 )
```

```
evecs = Eigenvectors[aTa];
% // MatrixForm

( -1  1
   1  1 )
```

■ Construct V.

The columns of the matrix V are the orthonormal eigenvectors of $A^T\ A$, taken in the proper order.

```
v1 = evecs[[1]] / Norm[evecs[[1]]];
v2 = evecs[[2]] / Norm[evecs[[2]]];

V = Transpose[{v1, v2}];
% // MatrixForm
```

$$\begin{pmatrix} -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix}$$

Check that the columns of V are orthonormal.

```
Transpose[V].V;
% // MatrixForm
```

$$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

Check the diagonalization.

```
aTa == V.Λ.Inverse[V]

True
```

■ Construct Σ .

```
<< LinearAlgebra`MatrixManipulation`
```

```
singularValues = {σ1, σ2} = √evals

Σ = ZeroMatrix[3, 2];
Σ[[1, 1]] = σ1;
Σ // MatrixForm
```

$\{3\sqrt{2}, 0\}$

$$\begin{pmatrix} 3\sqrt{2} & 0 \\ 0 & 0 \\ 0 & 0 \end{pmatrix}$$

■ Construct U .

Calculate u1

```
u1 = (1 / σ1) a.v1
```

$\left\{-\frac{1}{3}, \frac{2}{3}, -\frac{2}{3}\right\}$

Extend {u1} to an orthonormal basis of R^3.

```
u1 = (1 / σ1) a.v1;

e1 = {1, 0, 0};
f1 = (e1 - e1.u1 u1);
u2 = f1 / Norm[f1];

e2 = {0, 1, 0};
f2 = (e2 - e2.u1 u1 - e2.u2 u2);
u3 = f2 / Norm[f2];

U = Transpose[{u1, u2, u3}];
% // MatrixForm
```

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

Check that the columns of U are orthonormal.

```
Transpose[U].U;
% // MatrixForm
```

$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

■ Check the singular value decomposition, A == U.Σ.V^T.

```
Print[a // MatrixForm, "==", U // MatrixForm,
  ".", Σ // MatrixForm, ".", Transpose[V] // MatrixForm];
a == U.Σ.Transpose[V]
```

$$\begin{pmatrix} 1 & -1 \\ -2 & 2 \\ 2 & -2 \end{pmatrix} == \begin{pmatrix} -\frac{1}{3} & \frac{2\sqrt{2}}{3} & 0 \\ \frac{2}{3} & \frac{1}{3\sqrt{2}} & \frac{1}{\sqrt{2}} \\ -\frac{2}{3} & -\frac{1}{3\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix} . \begin{pmatrix} 3\sqrt{2} & 0 \\ 0 & 0 \\ 0 & 0 \end{pmatrix} . \begin{pmatrix} -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix}$$

```
True
```

■ Compare with *Mathematica*'s singular value decomposition.

Mathematica's numerical result.

```
a = ( 1.  -1
      -2   2
       2  -2 );

{u, w, v} = SingularValueDecomposition[a];

Print[a // MatrixForm, "==", u // MatrixForm,
  ".", w // MatrixForm, ".", Transpose[v] // MatrixForm];
a == u.w.Transpose[v]
```

$$\begin{pmatrix} 1. & -1 \\ -2 & 2 \\ 2 & -2 \end{pmatrix} == \begin{pmatrix} -0.333333 & 0.942809 & -7.40149\times 10^{-17} \\ 0.666667 & 0.235702 & 0.707107 \\ -0.666667 & -0.235702 & 0.707107 \end{pmatrix}$$

$$.\begin{pmatrix} 4.24264 & 0. \\ 0. & 0. \\ 0. & 0. \end{pmatrix}.\begin{pmatrix} -0.707107 & 0.707107 \\ 0.707107 & 0.707107 \end{pmatrix}$$

```
True
```

Our numerical result.
These agree up to the precision of the computer arithmetic that is involved.

```
Print[a // MatrixForm, "==", U // MatrixForm // N, ".",
  Σ // MatrixForm // N, ".", Transpose[V] // MatrixForm // N];
a == U.Σ.Transpose[V]
```

$$\begin{pmatrix} 1. & -1 \\ -2 & 2 \\ 2 & -2 \end{pmatrix} == \begin{pmatrix} -0.333333 & 0.942809 & 0. \\ 0.666667 & 0.235702 & 0.707107 \\ -0.666667 & -0.235702 & 0.707107 \end{pmatrix}$$

$$.\begin{pmatrix} 4.24264 & 0. \\ 0. & 0. \\ 0. & 0. \end{pmatrix}.\begin{pmatrix} -0.707107 & 0.707107 \\ 0.707107 & 0.707107 \end{pmatrix}$$

```
True
```

The Four Fundamental Subspaces

Consider the matrix of the previous example, ...

$$a = \begin{pmatrix} 1 & -1 \\ -2 & 2 \\ 2 & -2 \end{pmatrix};$$

... and its singular value decomposition, A == U.Σ.V^T.

```
Print[a // MatrixForm, "==", U // MatrixForm,
  ".", Σ // MatrixForm, ".", Transpose[V] // MatrixForm];

a == U.Σ.Transpose[V]
```

$$\begin{pmatrix} 1 & -1 \\ -2 & 2 \\ 2 & -2 \end{pmatrix} == \begin{pmatrix} -\frac{1}{3} & \frac{2\sqrt{2}}{3} & 0 \\ \frac{2}{3} & \frac{1}{3\sqrt{2}} & \frac{1}{\sqrt{2}} \\ -\frac{2}{3} & -\frac{1}{3\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix} . \begin{pmatrix} 3\sqrt{2} & 0 \\ 0 & 0 \\ 0 & 0 \end{pmatrix} . \begin{pmatrix} -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix}$$

```
True
```

a is an mxn matrix with rank r.

```
m = 3;
n = 2;
r = 1;
```

The **singular value decomposition** of a displays **orthogonal bases** for the **four fundamental subspaces** of a as follows:
(See Lay 7.4, p479)

```
(* α == [v1] == [v_1,...,v_r]   == basis for Row a *)
(* β == [v2] == [v_{r+1},...,v_n] == basis for Nul a *)

(* γ == [u1]    == [u_1,...,u_r]   == basis for Row a^T == Col a *)
(* δ == [u2,u3] == [u_{r+1},...,u_m] == basis for Nul a^T *)
```

The Moore-Penrose Inverse and Least-Squares Solutions

Consider the matrix of the previous example, ...

$$a = \begin{pmatrix} 1 & -1 \\ -2 & 2 \\ 2 & -2 \end{pmatrix};$$

... and its singular value decomposition, A == U.Σ.V^T.

```
Print[a // MatrixForm, "==", U // MatrixForm,
  ".", Σ // MatrixForm, ".", Transpose[V] // MatrixForm];

a == U.Σ.Transpose[V]
```

$$\begin{pmatrix} 1 & -1 \\ -2 & 2 \\ 2 & -2 \end{pmatrix} == \begin{pmatrix} -\frac{1}{3} & \frac{2\sqrt{2}}{3} & 0 \\ \frac{2}{3} & \frac{1}{3\sqrt{2}} & \frac{1}{\sqrt{2}} \\ -\frac{2}{3} & -\frac{1}{3\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix} . \begin{pmatrix} 3\sqrt{2} & 0 \\ 0 & 0 \\ 0 & 0 \end{pmatrix} . \begin{pmatrix} -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix}$$

```
True
```

a is an mxn matrix with rank r.

```
m = 3;
n = 2;
r = 1;
```

The **Moore-Penrose Inverse, A+,** or **pseudoinverse** of A is computed from its singular value decomposition, A == U.Σ.V^T, as follows:
(See Lay 7.4, p479)

```
Ur = Map[List, U[[All, 1]]];
Dr = {{σ1}};
Vr = Map[List, V[[All, 1]]];

aPlus = Vr.Inverse[Dr].Transpose[Ur];

Print[aPlus // MatrixForm, " == ", Vr // MatrixForm, ".",
  Inverse[Dr] // MatrixForm, ".", Transpose[Ur] // MatrixForm];
```

$$\begin{pmatrix} \frac{1}{18} & -\frac{1}{9} & \frac{1}{9} \\ -\frac{1}{18} & \frac{1}{9} & -\frac{1}{9} \end{pmatrix} == \begin{pmatrix} -\frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix} . \begin{pmatrix} \frac{1}{3\sqrt{2}} \end{pmatrix} . \begin{pmatrix} -\frac{1}{3} & \frac{2}{3} & -\frac{2}{3} \end{pmatrix}$$

Suppose we wish to solve the least-squares problem A.x == b.

```
(* a.x == b *)
```

Let

```
(* xHat = aPlus.b *)
```

Then,

```
(* a.xHat == (Ur.D.VrT).(Vr.D-1.UrT.b) ==
  (Ur.D.D-1.UrT.b) == Ur.UrT.b == bHat *)
```

where bHat is the orthogonal projection of b onto Col A == Col Ur.
Therefore, **xHat is a least squares solution of A.x == b**.

It can be shown that this xHat, obtained via the Moore-Penrose inverse of A,
is the **shortest least-squares solution** of A.x == b
(See Lay 7.4, p480)