

Singular Value Decomposition

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Theorem (SVD)

Any $m \times n$ matrix A , with $m \geq n$, can be factorized

$$A = U \begin{pmatrix} \Sigma \\ 0 \end{pmatrix} V^T, \quad (1)\text{span}$$

where $U \in \mathbb{R}^{m \times m}$ and $V \in \mathbb{R}^{n \times n}$ are orthogonal, and $\Sigma \in \mathbb{R}^{n \times n}$ is diagonal,

$$\begin{aligned} \Sigma &= \text{diag}(\sigma_1, \sigma_2, \dots, \sigma_n), \\ \sigma_1 &\geq \sigma_2 \geq \dots \geq \sigma_n \geq 0. \end{aligned}$$

$$\begin{matrix} \boxed{A} & = & \boxed{U} & \begin{matrix} \boxed{\begin{matrix} 0 \\ \diagdown \\ 0 \end{matrix}} & \boxed{V^T} \\ m \times n & & m \times m & m \times n & \end{matrix} \end{matrix}$$

Partition $U = (U_1 \ U_2)$, where $U_1 \in \mathbb{R}^{m \times n}$,

$$A = U_1 \Sigma V^T,$$

A $=$ U_1 Σ V^T

$m \times n$ $m \times n$ $n \times n$ $n \times n$

SVD Expansion

$$A = \sum_{i=1}^n \sigma_i u_i v_i^T = \begin{array}{|c} \text{---} \\ | \end{array} + \begin{array}{|c} \text{---} \\ | \end{array} + \dots$$

SVD of a matrix with full column rank I

```
A =  1    1
     1    2
     1    3
     1    4
```

```
>> [U,S,V]=svd(A)
```

```
U =  0.2195   -0.8073    0.0236    0.5472
     0.3833   -0.3912   -0.4393   -0.7120
     0.5472    0.0249    0.8079   -0.2176
     0.7110    0.4410   -0.3921    0.3824
```

```
S =  5.7794    0
     0    0.7738
     0    0
     0    0
```

SVD of a matrix with full column rank II

$$V = \begin{pmatrix} 0.3220 & -0.9467 \\ 0.9467 & 0.3220 \end{pmatrix}$$

```
>> [U,S,V]=svd(A,0)
```

```
U = 0.2195    -0.8073  
     0.3833    -0.3912  
     0.5472     0.0249  
     0.7110     0.4410
```

```
S = 5.7794     0  
     0     0.7738
```

```
V = 0.3220    -0.9467  
     0.9467     0.3220
```


Rank deficient matrix I

```
>> A(:,3)=A(:,1)+0.5*A(:,2)
```

```
A = 1.0000    1.0000    1.5000  
     1.0000    2.0000    2.0000  
     1.0000    3.0000    2.5000  
     1.0000    4.0000    3.0000
```

```
>> [U,S,V]=svd(A,0)
```

```
U = 0.2612   -0.7948   -0.5000  
     0.4032   -0.3708    0.8333  
     0.5451    0.0533   -0.1667  
     0.6871    0.4774   -0.1667
```

Rank deficient matrix II

$$S = \begin{bmatrix} 7.3944 & 0 & 0 \\ 0 & 0.9072 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

$$V = \begin{bmatrix} 0.2565 & -0.6998 & 0.6667 \\ 0.7372 & 0.5877 & 0.3333 \\ 0.6251 & -0.4060 & -0.6667 \end{bmatrix}$$

The *range* of the matrix A :

$$\mathcal{R}(A) = \{y \mid y = Ax, \text{ for arbitrary } x\}.$$

Assume that A has rank r :

$$\sigma_1 \geq \cdots \geq \sigma_r > \sigma_{r+1} = \cdots = \sigma_n = 0.$$

Outer product form:

$$y = Ax = \sum_{i=1}^r \sigma_i u_i v_i^T x = \sum_{i=1}^r (\sigma_i v_i^T x) u_i = \sum_{i=1}^r \alpha_i u_i.$$

The *null-space* of the matrix A :

$$\mathcal{N}(A) = \{x \mid Ax = 0\}.$$

$$Ax = \sum_{i=1}^r \sigma_i u_i v_i^T x$$

Any vector $z = \sum_{i=r+1}^n \beta_i v_i$ is in the null-space:

$$Az = \left(\sum_{i=1}^r \sigma_i u_i v_i^T \right) \left(\sum_{i=r+1}^n \beta_i v_i \right) = 0.$$

Theorem (Fundamental subspaces)

- ① *The singular vectors u_1, u_2, \dots, u_r are an orthonormal basis in $\mathcal{R}(A)$ and*

$$\text{rank}(A) = \dim(\mathcal{R}(A)) = r.$$

- ② *The singular vectors $v_{r+1}, v_{r+2}, \dots, v_n$ are an orthonormal basis in $\mathcal{N}(A)$ and*

$$\dim(\mathcal{N}(A)) = n - r.$$

- ③ *The singular vectors v_1, v_2, \dots, v_r are an orthonormal basis in $\mathcal{R}(A^T)$.*
- ④ *The singular vectors $u_{r+1}, u_{r+2}, \dots, u_m$ are an orthonormal basis in $\mathcal{N}(A^T)$.*

The third column of V is a basis vector in $N(A)$:

```
>> A*V(:,3)
```

```
ans =
```

```
1.0e-15 *  
    0  
-0.2220  
-0.2220  
    0
```

Frobenius norm

$$\|A\|_F = \left(\sum_{i,j} a_{ij}^2 \right)^{1/2}$$

Theorem

Assume that the matrix $A \in \mathbb{R}^{m \times n}$ has rank $r > k$. The Frobenius norm matrix approximation problem

$$\min_{\text{rank}(Z)=k} \|A - Z\|_F$$

has the solution

$$Z = A_k = U_k \Sigma_k V_k^T,$$

Principal Component Analysis (PCA) I

Data matrix $\mathbb{R}^{m \times n} \ni X = U\Sigma V^T$

Each column is an observation of a real-valued random vector with mean zero.

The right singular vectors v_i are called **principal components directions** of X . The vector

$$z_1 = Xv_1 = \sigma_1 u_1$$

has the largest sample variance amongst all normalized linear combinations of the columns of X :

$$\text{Var}(z_1) = \text{Var}(Xv_1) = \frac{\sigma_1^2}{m}.$$

The normalized variable u_1 is called the **normalized first principal component** of X . The second principal component is the vector of largest sample variance of the deflated data matrix $X - \sigma_1 u_1 v_1^T$, and so on.

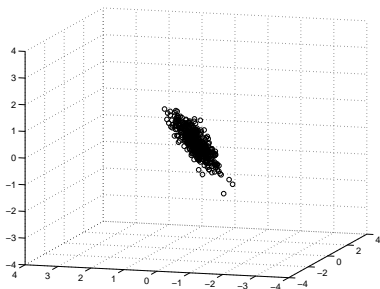
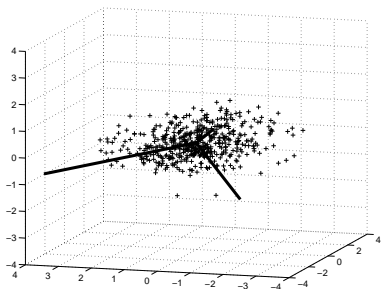


Figure: Cluster of points in \mathbb{R}^3 with (scaled) principal components (top). The same data with the contributions along the first principal component deflated (bottom).

Least Squares by SVD I

```
A =  1    1
     1    2
     1    3
     1    4
     1    5

b =  7.9700
     10.2000
     14.2000
     16.0000
     21.2000
```

```
>> [U1,S,V]=svd(A,0)
```

```
U1 =0.1600   -0.7579
     0.2853   -0.4675
     0.4106   -0.1772
     0.5359    0.1131
     0.6612    0.4035
```

Least Squares by SVD II

```
S = 7.6912      0
      0      0.9194
```

```
V = 0.2669    -0.9637
      0.9637    0.2669
```

```
>> x=V*(S\u1' * b))
```

```
x = 4.2360
      3.2260
```

Least Squares by SVD, in R |

```
> A.svd<-svd(A)
> A.svd
$d
[1] 7.6912131 0.9193696

$u
      [,1]      [,2]
[1,] 0.1600071 0.7578903
[2,] 0.2853078 0.4675462
[3,] 0.4106086 0.1772020
[4,] 0.5359094 -0.1131421
[5,] 0.6612102 -0.4034862

$v
      [,1]      [,2]
```

Least Squares by SVD, in R II

```
[1,] 0.2669336  0.9637149  
[2,] 0.9637149 -0.2669336
```

```
> x=A.svd$v %*% diag(1/A.svd$d) %*% t(A.svd$u) %*% b
```

```
> x
```

```
      [,1]  
[1,] 4.236  
[2,] 3.226
```

```
>
```

Theorem

Let the singular values of A satisfy

$$\sigma_1 \geq \cdots \geq \sigma_r > \sigma_{r+1} = \cdots = \sigma_n = 0.$$

Then the rank of A is equal to r .

Rank = the number of linearly independent columns of A .

Linear dependence I

```
A=[1 1; 1 2; 1 3; 1 4]
singval=svd(A)
```

```
% Third col=linear combination of first two
A1=[A A(:,1)+0.5*A(:,2)]
singval1=svd(A1)
```

```
A =   1   1
      1   2
      1   3
      1   4
```

Result:

Linear dependence II

```
singval = 5.7794  
         0.7738
```

```
A1 = 1.0000    1.0000    1.5000  
     1.0000    2.0000    2.0000  
     1.0000    3.0000    2.5000  
     1.0000    4.0000    3.0000
```

```
singval1 = 7.3944  
          0.9072  
          0
```


Almost linear dependence I

```
A2=[A A(:,1)+0.5*A(:,2)+0.0001*randn(4,1)]
```

```
singval2=svd(A2)
```

```
A2 = 1.0000    1.0000    1.4999  
      1.0000    2.0000    2.0001  
      1.0000    3.0000    2.5000  
      1.0000    4.0000    3.0001
```

```
singval2 = 7.3944  
           0.9072  
           0.0001
```