Chapter 6

Singular Value Decomposition

Even if the QR decomposition is very useful for solving least squares problems, and has excellent stability properties, it has the drawback that it treats the rows and columns of the matrix differently: It only gives a basis for the *column space.* The singular value decomposition (SVD) deals with the rows and columns in a symmetric fashion, and therefore it supplies more information about the matrix. It also "orders" the information contained in the matrix so that, loosely speaking, the "dominating part" becomes visible. This is the property that makes the SVD so useful in data mining and may other areas.

6.1 The Decomposition

Theorem 6.1 (SVD). *Any $m \times n$ matrix A, with $m \geq n$, can be factorized*

$$A = U \begin{pmatrix} \Sigma \\ 0 \end{pmatrix} V^T, \tag{6.1}$$

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

$$\Sigma = \operatorname{diag}(\sigma_1, \sigma_2, \ldots, \sigma_n),$$

$$\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_n \geq 0.$$

Proof. The assumption $m \geq n$ is no restriction: in the other case, just apply the theorem to A^T.

We give a proof along the lines of that in [36]. Consider the maximization problem

$$\sup_{\|x\|_2=1} \|Ax\|_2.$$

Since we are seeking the supremum of a continuous function over a closed set, the supremum is attained for some vector x. Put $Ax = \sigma_1 y$, where $\|y\|_2 = 1$ and

$\sigma_1 = \| A \|_2$ (by definition). Using Proposition 4.7 we can construct orthogonal matrices

$$Z_1 = (y\, \bar{Z}_2) \in \mathbb{R}^{m\times m}, \quad W_1 = (x\, \bar{W}_2) \in \mathbb{R}^{n\times n}.$$

Then

$$Z_1^T A W_1 = \begin{pmatrix} \sigma_1 & y^T A \bar{W}_2 \\ 0 & \bar{Z}_2^T A \bar{W}_2 \end{pmatrix},$$

since $y^T A x = \sigma_1$, and $Z_2^T A x = \sigma_1 \bar{Z}_2^T y = 0$. Put

$$A_1 = Z_1^T A W_1 = \begin{pmatrix} \sigma_1 & w^T \\ 0 & B \end{pmatrix}.$$

Then

$$\frac{1}{\sigma_1^2 + w^T w} \left\| A_1 \begin{pmatrix} \sigma_1 \\ w \end{pmatrix} \right\|_2^2 = \frac{1}{\sigma_1^2 + w^T w} \left\| \begin{pmatrix} \sigma_1^2 + w^T w \\ Bw \end{pmatrix} \right\|_2^2 \geq \sigma_1^2 + w^T w.$$

But $\| A_1 \|_2^2 = \| Z_1^T A W_1 \|_2^2 = \sigma_1^2$; therefore $w = 0$ must hold. Thus we have taken one step towards a diagonalization of A. The proof is now completed by induction: Assume that

$$B = Z_2 \begin{pmatrix} \Sigma_2 \\ 0 \end{pmatrix} W_2, \quad \Sigma_2 = \mathrm{diag}(\sigma_2, \ldots, \sigma_n).$$

Then we have

$$A = Z_1 \begin{pmatrix} \sigma_1 & 0 \\ 0 & B \end{pmatrix} W_1^T = Z_1 \begin{pmatrix} 1 & 0 \\ 0 & Z_2 \end{pmatrix} \begin{pmatrix} \sigma_1 & 0 \\ 0 & \Sigma_2 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & W_2^T \end{pmatrix} W_1^T.$$

Thus, the theorem follows with

$$U = Z_1 \begin{pmatrix} 1 & 0 \\ 0 & Z_2 \end{pmatrix}, \quad \Sigma = \begin{pmatrix} \sigma_1 & 0 \\ 0 & \Sigma_2 \end{pmatrix}, \quad V = W_1 \begin{pmatrix} 1 & 0 \\ 0 & W_2 \end{pmatrix}.$$

□

The columns of U and V are called *singular vectors* and the diagonal elements σ_i *singular values.*

We emphasize at this point that not only is this an important theoretical result, but also there are very efficient and accurate algorithms for computing the SVD, cf. Section 6.9.

The SVD appears in other scientific areas under different names. In statistics and data analysis the singular vectors are closely related to *principal components*, see Section 6.4. and in image processing the SVD goes under the name of *Karhunen-Loewe expansion.*

We illustrate the SVD symbolically in Figure 6.1.

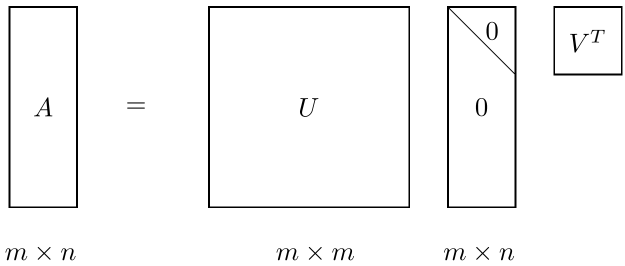

Figure 6.1. *Symbolic illustration of the singular value decomposition.*

With the partitioning $U = (U_1 \, U_2)$, where $U_1 \in \mathbb{R}m \times n$, we get the "thin version" of the SVD,

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

We illustrate the thin SVD symbolically in Figure 6.2.

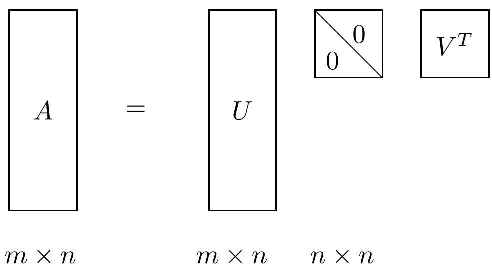

Figure 6.2. *Symbolic illustration of the thin SVD.*

If we write out the matrix equations

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

column by column, we get the equivalent equations

$$Av_i = \sigma_i u_i, \qquad A^T u_i = \sigma_i v_i, \qquad i = 1, 2, \ldots, n.$$

The SVD can also be written as an expansion of the matrix:

$$A = \sum_{i=1}^{n} \sigma_i u_i v_i^T. \tag{6.2}$$

This is usually called the *outer product form*, and it is derived by starting from the thin version:

$$A = U_1 \Sigma V^T = \begin{pmatrix} u_1 & u_2 & \cdots & u_n \end{pmatrix} \begin{pmatrix} \sigma_1 & & & \\ & \sigma_2 & & \\ & & \ddots & \\ & & & \sigma_n \end{pmatrix} \begin{pmatrix} v_1^T \\ v_2^T \\ \vdots \\ \sigma_n \end{pmatrix}$$

$$= \begin{pmatrix} u_1 & u_2 & \cdots & u_n \end{pmatrix} \begin{pmatrix} \sigma_1 v_1^T \\ \sigma_2 v_2^T \\ \vdots \\ \sigma_n \sigma_n \end{pmatrix} = \sum_{i=1}^{n} \sigma_i u_i v_i^T.$$

The outer product form of the SVD is illustrated in Figure 6.3.

$$A = \sum_{i=1}^{n} \sigma_i u_i v_i^T =$$

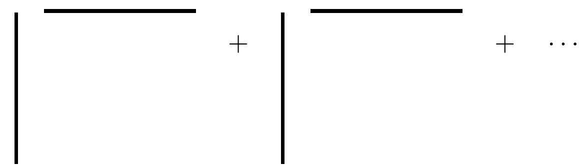

Figure 6.3. *The SVD as a sum of rank one matrices.*

Example 6.2 We illustrate with the SVD of a matrix with full column rank:

```
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

V = 0.3220   -0.9467
    0.9467    0.3220
```

The thin version of the SVD is

```
>> [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
```

■

The matrix 2-norm was defined in Section 2.4. From the proof of Theorem 6.1 we know already that $\| A \|_2 = \sigma_1$. This is such an important fact that it is worth a separate proposition.

Proposition 6.3. *The 2-norm of a matrix is given by*

$$\| A \|_2 = \sigma_1.$$

Proof. The following is an alternative proof. Let the SVD of A be $A = U\Sigma V^T$. Since the norm is invariant under orthogonal transformations, we see that

$$\| A \|_2 = \| \Sigma \|_2.$$

The result now follows, since the 2-norm of a diagonal matrix is equal to the absolute value of the largest element, cf. Exercise 3. □

6.2 Fundamental Subspaces

The SVD gives orthogonal bases of the four fundamental subspaces of a matrix.

The *range of the matrix* A is the linear subspace

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

Assume that A has rank r:

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

Then, using the outer product form, we have

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

The *null-space of the matrix* A is the linear subspace

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

Since $Ax = \sum_{i=1}^{r} \sigma_i u_i v_i^T x$, we see that any vector $z = \sum_{i=r+1}^{n} \beta_i v_i$ is in the null-space:

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

After a similar demonstration for A^T we have the following theorem.

Theorem 6.4 (Fundamental subspaces).

1. *The singular vectors* $u_1, u_2, \ldots, u_r$ *are an orthonormal basis in* $\mathcal{R}(A)$ *and*
$$\text{rank}(A) = \dim(\mathcal{R}(A)) = r.$$
2. *The singular vectors* $v_{r+1}, v_{r+2}, \ldots, v_n$ *are an orthonormal basis in* $\mathcal{N}(A)$ *and*
$$\dim(\mathcal{N}(A)) = n - r.$$
3. *The singular vectors* $v_1, v_2, \ldots, v_r$ *are an orthonormal basis in* $\mathcal{R}(A^T)$.
4. *The singular vectors* $u_{r+1}, u_{r+2}, \ldots, u_m$ *are an orthonormal basis in* $\mathcal{N}(A^T)$.

Example 6.5 We create a rank deficient matrix by constructing a third column in the previous example as a linear combination of columns 1 and 2:

```
>> 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

S = 7.3944         0         0
         0    0.9072         0
         0         0         0

V = 0.2565   -0.6998    0.6667
    0.7372    0.5877    0.3333
    0.6251   -0.4060   -0.6667
```

The third singular value is equal to zero and the matrix is rank deficient. Obviously, the third column of `V` is a basis vector in $\mathcal{N}(A)$:

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

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

■

6.3 Matrix Approximation

Assume that A is a low rank matrix plus noise: $A = A_0 + N$, where the noise N is small compared to A_0. Then typically the singular values of A have the behaviour illustrated in Figure 6.4. In such a situation, if the noise is significantly smaller in

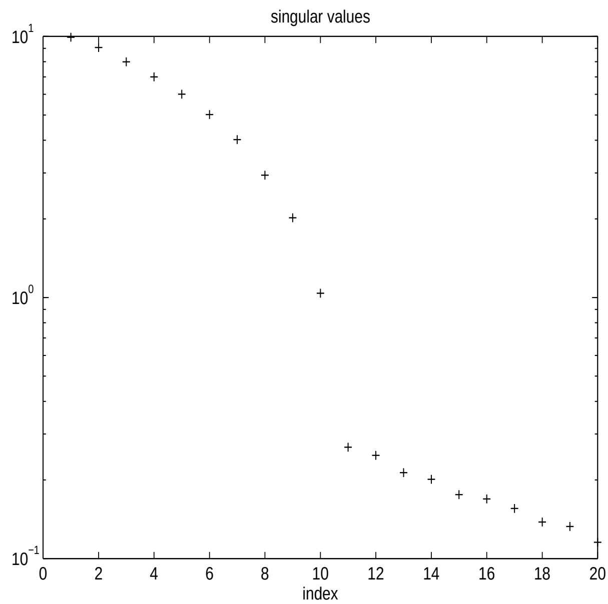

Figure 6.4. *Singular values of a matrix of rank 10 plus noise.*

magnitude, the number of large singular values is often referred to as the *numerical rank* of the matrix. If we know the correct rank of A_0, or can estimate it, e.g. by inspecting the singular values, then we can "remove the noise" by approximating A by a matrix of the correct rank. The obvious way to do this is simply to truncate the singular value expansion (6.2). Assume that the numerical rank is equal to k. Then we approximate

$$A = \sum_{i=1}^{n} \sigma_i u_i v_i^T \approx \sum_{i=1}^{k} \sigma_i u_i v_i^T =: A_k.$$

The truncated SVD is very important, not only for removing noise, but also for compressing data, see Chapter 12, and for stabilizing the solution of problems that are extremely ill-conditioned.

It turns out that the truncated SVD is the solution of approximation problems, where one wants to approximate a given matrix by one of lower rank. We will consider low-rank approximation of a matrix A in two norms. First we give the theorem for the matrix 2-norm.

Theorem 6.6. *Assume that the matrix $A \in \mathbb{R}^{m\times n}$ has rank $r > k$. The matrix approximation problem*

$$\min_{\operatorname{rank}(Z)=k} \|A - Z\|_2$$

has the solution

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

where $U_k = (u_1, \ldots, u_k)$, $V_k = (v_1, \ldots, v_k)$ and $\Sigma_k = \operatorname{diag}(\sigma_1, \ldots, \sigma_k)$. The minimum is

$$\|A - A_k\|_2 = \sigma_{k+1}.$$

A proof of this theorem can be found, e.g. in [36, Section 2.5.5]. Next recall the definition of the *Frobenius matrix norm* (2.6)

$$\|A\|_F = \sqrt{\sum_{i,j} a_{ij}^2}.$$

It turns out that the approximation result is the same for this case.

Theorem 6.7. *Assume that the matrix $A \in \mathbb{R}^{m\times n}$ has rank $r > k$. The Frobenius norm matrix approximation problem*

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

has the solution

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

where $U_k = (u_1, \ldots, u_k)$, $V_k = (v_1, \ldots, v_k)$ and $\Sigma_k = \operatorname{diag}(\sigma_1, \ldots, \sigma_k)$. The minimum is

$$\|A - A_k\|_F = \left(\sum_{i=k+1}^{p} \sigma_i^2 \right)^{1/2},$$

where $p = \min(m, n)$.

For the proof of this theorem we need a lemma.

Lemma 6.8. *Consider the mn-dimensional vector space $\mathbb{R}^{m\times n}$ with inner product*

$$\langle A, B\rangle = \operatorname{tr}(A^T B) = \sum_{i=1}^{m}\sum_{j=1}^{n} a_{ij} b_{ij}, \tag{6.3}$$

and norm

$$\|A\|_F = \langle A, A\rangle^{1/2}.$$

Let $A \in \mathbb{R}^{m\times n}$ with SVD $A = U\Sigma V^T$. Then the matrices

$$u_i v_j^T, \qquad i = 1, 2, \ldots, m, \qquad j = 1, 2, \ldots, n, \tag{6.4}$$

are an orthonormal basis in $\mathbb{R}^{m\times n}$.

Proof. Using the identities $\langle A, B\rangle = \mathrm{tr}(A^T B) = \mathrm{tr}(BA^T)$ we get

$$\langle u_i v_j^T, u_k v_l^T\rangle = \mathrm{tr}(v_j u_i^T u_k v_l^T) = \mathrm{tr}(v_l^T v_j\, u_i^T u_k) = (v_l^T v_j)\,(u_i^T u_k),$$

which shows that the matrices are orthonormal. Since there are mn such matrices, they constitute a basis in $\mathbb{R}^{m\times n}$. $\square$

Proof. (**Theorem** (6.7). The proof is essentially the same as in [35].) Write the matrix $Z \in \mathbb{R}^{m\times n}$ in terms of the basis (6.4),

$$Z = \sum_{i,j} \zeta_{ij} u_i v_j^T,$$

where the coefficients are to be chosen. Since Z is assumed to have rank k, only k of the coefficients should be non-zero. For the purpose of this proof we denote the elements of Σ by σ_{ij}. Due to the orthonormality of the basis, we have

$$\|A - Z\|_F^2 = \sum_{i,j}(\sigma_{ij} - \zeta_{ij})^2 = \sum_i (\sigma_{ii} - \zeta_{ii})^2 + \sum_{i\neq j} \zeta_{ij}^2.$$

Obviously, we can choose the second term equal to zero, and to minimize the objective function, we should then choose

$$\zeta_{ii} = \sigma_{ii}, \quad i = 1, 2, \ldots, k,$$

which gives the desired result. $\square$

The low rank approximation of a matrix is illustrated in Figure 6.5.

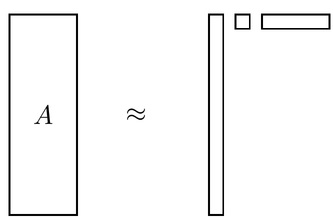

Figure 6.5. *Symbolic illustration of low rank approximation by SVD:* $A \approx A_k = U_k \Sigma_k V_k^T$.

6.4 Principal Component Analysis

The approximation properties of the SVD can be used to elucidate the equivalence between the SVD and *principal component analysis (PCA)*. Assume that $X \in$

$\mathbb{R}^{m\times n}$ is a data matrix, where each column is an observation of a real-valued random vector with mean zero. The matrix is assumed to be centered, i.e. the mean of each column is equal to zero. Let the SVD of X be $X = U\Sigma V^T$. The right singular vectors v_i are called *principal components directions* of X [43, p. 62]. 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:

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

Finding the vector of maximal variance is equivalent, using linear algebra terminology, to maximizing the Rayleigh quotient:

$$\sigma_1^2 = \max_{v\neq 0} \frac{v^T X^T X v}{v^T v}, \qquad v_1 = \arg\max_{v\neq 0} \frac{v^T X^T X v}{v^T v}.$$

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. Equivalently, any subsequent principal component is defined as the vector of maximal variance subject to the constraint that it is orthogonal to the previous ones.

Example 6.9 PCA is illustrated in Figure 6.6. 500 data points from a correlated normal distribution were generated, and collected in a data matrix $X \in \mathbb{R}^{3\times 500}$. The data points and the principal components are illustrated in the top plot. We then deflated the data matrix, $X_1 := X - \sigma_1 u_1 v_1^T$; the data points corresponding to X_1 are given in the bottom plot. ■

6.5 Solving Least Squares Problems

The least squares problem can be solved using the SVD. Assume that we have an over-determined system $Ax \sim b$, where the matrix A has full column rank. Write the SVD

$$A = (U_1\ U_2) \begin{pmatrix} \Sigma \\ 0 \end{pmatrix} V^T,$$

where $U_1 \in \mathbb{R}m \times n$. Then, using the SVD and the fact that the norm is invariant under orthogonal transformations

$$\|r\|^2 = \|b - Ax\|^2 = \left\| b - U \begin{pmatrix} \Sigma \\ 0 \end{pmatrix} V^T x \right\|^2 = \left\| \begin{pmatrix} b_1 \\ b_2 \end{pmatrix} - \begin{pmatrix} \Sigma \\ 0 \end{pmatrix} y \right\|^2,$$

where $b_i = U_i^T b$ and $y = V^T x$. Thus

$$\|r\|^2 = \|b_1 - \Sigma y\|^2 + \|b_2\|^2.$$

We can now minimize $\|r\|^2$ by putting $y = \Sigma^{-1} b_1$. Then the solution is given by

$$x = Vy = V\Sigma^{-1} b_1 = V\Sigma^{-1} U_1^T b. \tag{6.5}$$

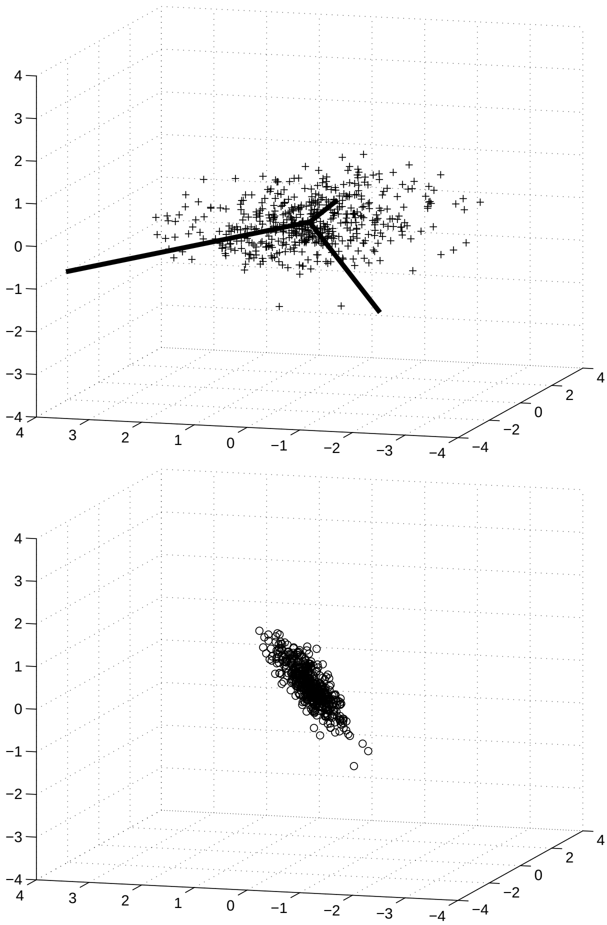

Figure 6.6. *Cluster of points in* $\mathbb{R}^3$ *with (scaled) principal components (top). The same data with the contributions along the first principal component deflated (bottom).*

Recall that Σ is diagonal,

$$\Sigma^{-1} = \mathrm{diag}(\frac{1}{\sigma_1}, \frac{1}{\sigma_2}, \ldots, \frac{1}{\sigma_n}),$$

so the solution can also be written

$$x = \sum_{i=1}^{n} \frac{u_i^T b}{\sigma_i} v_i.$$

Note that the assumption that A has full column rank rank implies that all the singular values are non-zero: $\sigma_i > 0$, $i = 1, 2, \ldots, n$. We also see that in this case, the solution is unique.

Theorem 6.10 (Least squares solution by SVD). *Let the matrix $A \in \mathbb{R}^{m\times n}$ have full column rank, and thin SVD $A = U_1 \Sigma V^T$. Then the least squares problem* $\min_x \| Ax - b \|_2$ *has the unique solution*

$$x = V\Sigma^{-1}U_1^T b = \sum_{i=1}^{n} \frac{u_i^T b}{\sigma_i} v_i.$$

Example 6.11 As an example, we solve the least squares problem given at the beginning of Chapter 3.6. The matrix and right hand side are

```
A =  1     1               b = 7.9700
     1     2                  10.2000
     1     3                  14.2000
     1     4                  16.0000
     1     5                  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

 S = 7.6912         0
          0    0.9194

 V = 0.2669   -0.9637
    0.9637    0.2669
```

It can be seen that the two column vectors in A are linearly independent since the singular values are both non-zero. The least squares problem is solved using (6.5)

```
>> x=V*(S\(U1'*b))

x = 4.2360
    3.2260
```

∎

6.6 Condition Number and Perturbation Theory for the Least Squares Problem

The condition number of a rectangular matrix is defined in terms of the singular value decomposition. Let A have rank r, i.e., its singular values satisfy

$$\sigma_1 \geq \cdots \geq \sigma_r > \sigma_{r+1} = \cdots = \sigma_p = 0,$$

where $p = \min(m, n)$. Then the condition number is defined

$$\kappa(A) = \frac{\sigma_1}{\sigma_r}.$$

Note that in the case of a square, nonsingular matrix, this reduces to the definition (3.3).

The following perturbation theorem was proved by Wedin [94].

Theorem 6.12. *Assume that the matrix $A \in \mathbb{R}^{m\times n}$, where $m \geq n$ has full column rank, and let x be the solution of the least squares problem $\min_x \| Ax - b \|_2$. Let δA and δb be perturbations such that*

$$\eta = \frac{\| \delta A \|_2}{\sigma_n} = \kappa \epsilon_A < 1, \qquad \epsilon_A = \frac{\| \delta A \|_2}{\| A \|_2}.$$

Then the perturbed matrix $A + \delta A$ has full rank, and the perturbation of the solution δx satisfies

$$\| \delta x \|_2 \leq \frac{\kappa}{1-\eta} \left(\epsilon_A \| x \|_2 + \frac{\| \delta b \|_2}{\| A \|_2} + \epsilon_A \kappa \frac{\| r \|_2}{\| A \|_2} \right),$$

where r is the residual $r = b - Ax$.

There are at least two important observations to make here:

1. The number κ determines the condition of the least squares problem, and if $m = n$, then the residual r is equal to zero and the inequality becomes a perturbation result for a linear system of equations, cf. Theorem 3.5.

2. In the over-determined case the residual is usually not equal to zero. Then the conditioning depends on κ^2. This may be significant if the norm of the residual is large.

6.7 Rank-Deficient and Under-determined Systems

Now assume that A is rank-deficient, i.e. $\operatorname{rank}(A) = r < \min(m, n)$. The least squares problem can still be solved, but the solution is no longer unique. In this case we can write the SVD

$$A = \begin{pmatrix} U_1 & U_2 \end{pmatrix} \begin{pmatrix} \Sigma_1 & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} V_1^T \\ V_2^T \end{pmatrix}, \tag{6.6}$$

where

$$U_1 \in \mathbb{R}^{m\times r}, \qquad \Sigma_{\in} \mathbb{R}^{r\times r}, \qquad V_1 \in \mathbb{R}^{n\times r}, \tag{6.7}$$

and the diagonal elements of Σ_1 are all non-zero. The norm of the residual can now be written

$$\| r \|_2^2 = \| Ax - b \|_2^2 = \left\| \begin{pmatrix} U_1 & U_2 \end{pmatrix} \begin{pmatrix} \Sigma_1 & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} V_1^T \\ V_2^T \end{pmatrix} x - b \right\|_2^2.$$

Putting

$$y = V^T x = \begin{pmatrix} V_1^T x \\ V_2^T x \end{pmatrix} = \begin{pmatrix} y_1 \\ y_2 \end{pmatrix}, \qquad \begin{pmatrix} b_1 \\ b_2 \end{pmatrix} = \begin{pmatrix} U_1^T b \\ U_2^T b \end{pmatrix},$$

and using the invariance of the norm under orthogonal transformations, the residual becomes

$$\| r \|_2^2 = \left\| \begin{pmatrix} \Sigma_1 & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} y_1 \\ y_2 \end{pmatrix} - \begin{pmatrix} b_1 \\ b_2 \end{pmatrix} \right\|_2^2 = \| \Sigma_1 y_1 - b_1 \|_2^2 + \| b_2 \|_2^2.$$

Thus, we can minimize the residual by choosing $y_1 = \Sigma_1^{-1} b_1$. In fact,

$$y = \begin{pmatrix} \Sigma_1^{-1} b_1 \\ y_2 \end{pmatrix}$$

where y_2 is arbitrary, solves the least squares problem. Therefore, *the solution of the least squares problem is not unique*, and, since the columns of V_2 span the null-space of A, it is in this null-space, where the indeterminacy is. We can write

$$\| x \|_2^2 = \| y \|_2^2 = \| y_1 \|_2^2 + \| y_2 \|_2^2,$$

and therefore we obtain the solution of *minimum norm* by choosing $y_2 = 0$.

We summarize the derivation in a theorem.

Theorem 6.13 (Minimum norm solution). *Assume that the matrix A is rank deficient with SVD (6.6), (6.7). Then the least squares problem $\min_x \| Ax - b \|_2$ does not have a unique solution. However, the problem*

$$\min_{x \in \mathcal{L}} \| x \|_2, \qquad \mathcal{L} = \{ x \mid \| Ax - b \|_2 = \min \},$$

has the unique solution

$$x = V \begin{pmatrix} \Sigma_1^{-1} & 0 \\ 0 & 0 \end{pmatrix} U^T b = V_1 \Sigma_1^{-1} U_1^T b.$$

The matrix

$$A^\dagger = V \begin{pmatrix} \Sigma_1^{-1} & 0 \\ 0 & 0 \end{pmatrix} U^T,$$

is called the *pseudoinverse* of A. It is defined for any non-zero matrix of arbitrary dimensions.

The SVD can also be used to solve *under-determined linear systems*, i.e. systems with more unknowns than equations. The SVD of such a matrix is give by

$$\mathbb{R}^{m \times n} \ni A = U \begin{pmatrix} \Sigma & 0 \end{pmatrix} \begin{pmatrix} V_1^T \\ V_2^T \end{pmatrix}, \qquad V_1 \in \mathbb{R}^{m \times m}. \tag{6.8}$$

Obviously A has full row rank if and only Σ is nonsingular.

We state a theorem concerning the solution of a linear system

$$Ax = b, \tag{6.9}$$

for the case when A has full row rank. The rank deficient case may or may not have a solution depending in the right hand side, and that case can be easily treated as in Theorem 6.13.

Theorem 6.14 (Solution of an under-determined linear system). *Let $A \in \mathbb{R}^{m\times n}$ have full row rank with SVD* (6.8)*. Then the linear system* (6.9) *always has a solution, which, however, is non-unique. The problem*

$$\min_{x\in\mathcal{K}} \| x \|_2, \qquad \mathcal{K} = \{x \mid Ax = b\}, \tag{6.10}$$

has the unique solution

$$x = V_1^T \Sigma^{-1} U^T b. \tag{6.11}$$

Proof. Using the SVD (6.8) we can write

$$Ax = U \begin{pmatrix} \Sigma & 0 \end{pmatrix} \begin{pmatrix} V_1^T x \\ V_2^T x \end{pmatrix} =: U \begin{pmatrix} \Sigma & 0 \end{pmatrix} \begin{pmatrix} y_1 \\ y_2 \end{pmatrix} = U\Sigma y_1.$$

Since Σ is nonsingular, we see that for any right hand side, (6.11) is a solution of the linear system. However, we can add an arbitrary solution component in the null-space of A, $y_2 = V_2^T x$, and we still have a solution. The minimum norm solution, i.e. the solution of (6.10), is given by (6.11). □

6.8 Generalized SVD

We have seen that the SVD can be used to solve linear equations and least squares problems. Quite often generalizations of least squares problems occur, involving two matrices. An example is the linear least squares problem with a linear equality constraint

$$\min_x \| Ax - c \|_2, \quad \text{subject to} \quad Bx = d. \tag{6.12}$$

Other problems involving two matrices will occur in Chapter 12.

Such problems can be analyzed and solved using a simultaneous diagonalization of the two matrices, the generalized SVD.

Theorem 6.15 (Generalized SVD). *Let $A \in \mathbb{R}^{m\times n}$, $m \geq n$, and $B \in \mathbb{R}^{p\times n}$. Then there exist orthogonal matrices $U \in \mathbb{R}^{m\times m}$ and $V \in \mathbb{R}^{p\times p}$, and a nonsingular $X \in \mathbb{R}^{n\times n}$, such that*

$$U^T AX = C = \operatorname{diag}(c_1, \ldots, c_n), \quad 0 \leq c_1 \leq \cdots \leq c_n \leq 1, \tag{6.13}$$

$$V^T BX = S = \operatorname{diag}(s_1, \ldots, s_q), \quad 1 \geq s_1 \geq \cdots \geq s_q \geq 0, \tag{6.14}$$

where $q = \min(p, n)$ *and*

$$C^T C + S^T S = I.$$

Proof. A proof can be found in [36, Section 8.7.3], see also [89, 66]. ∎

The generalized SVD is sometimes called the Quotient SVD. There is also a different generalization, called the *Product SVD*, see e.g. [23, 38].

We will now show how we can solve the least squares problem with equality constraints (6.12). For simplicity we assume that the following assumption holds,

$$\mathcal{N}(A) \cap \mathcal{N}(B) = \{0\}; \tag{6.15}$$

(otherwise the solution would not be unique). We further assume that the constraint has a full row rank matrix B, which has fewer rows than columns (otherwise, if A is square and full rank, the least squares part of (6.12) is vacuous). The GSVD can be written

$$A = U \begin{pmatrix} C \\ 0 \end{pmatrix} X^{-1}$$
$$B = V \begin{pmatrix} S & 0 \end{pmatrix} X^{-1},$$

where, due to the assumption that B has full row rank, the matrix S is nonsingular. With

$$y = X^{-1} x = \begin{pmatrix} y_1 \\ y_2 \end{pmatrix}, \quad y_1 \in \mathbb{R}^p,$$

the constraint becomes

$$d = V \begin{pmatrix} S & 0 \end{pmatrix} \begin{pmatrix} y_1 \\ y_2 \end{pmatrix} = V S y_1,$$

which is satisfied by putting

$$y_1 = S^{-1} V^T d. \tag{6.16}$$

It remains to determine y_2 using the least squares problem. Using the orthogonal invariance of the norm we get the residual

$$\| r \|_2^2 = \left\| \begin{pmatrix} C \\ 0 \end{pmatrix} \begin{pmatrix} y_1 \\ y_2 \end{pmatrix} - U^T c \right\|_2^2 .$$

Partitioning

$$C = \begin{pmatrix} C_1 & 0 \\ 0 & C_2 \end{pmatrix}, \quad C_1 \in \mathbb{R}^{p \times p}, \tag{6.17}$$

we first see that, due to the assumption (6.15), the diagonal matrix C_2 must be nonsingular (cf. Exercise 3). Then, with the partitioning of U and $U^T c$,

$$U = \begin{pmatrix} U_1 & U_2 & U_3 \end{pmatrix}, \qquad U^T c = \begin{pmatrix} c_1 \\ c_2 \\ c_3 \end{pmatrix} = \begin{pmatrix} U_1^T c \\ U_2^T c \\ U_3^T c \end{pmatrix},$$

Decomposition	flops
LU	$2n^3/3$
QR (Householder)	$4n^3/3$
QR (plane rot.)	$8n^3/3$
SVD	$\leq 10n^3$

Table 6.1. *Flop counts for matrix decompositions.*

where $U_1 \in \mathbb{R}^{m\times p}$, and $U_2 \in \mathbb{R}^{m\times(n-p)}$, we can write the residual

$$\begin{aligned} \| r \|_2^2 &= \left\| \begin{pmatrix} C_1 & 0 \\ 0 & C_2 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} y_1 \\ y_2 \end{pmatrix} - \begin{pmatrix} c_1 \\ c_2 \\ c_3 \end{pmatrix} \right\|_2^2 \\ &= \| C_1 y_1 - c_1 \|_2^2 + \| C_2 y_2 - c_2 \|_2^2 + \| c_3 \|_2^2, \end{aligned}$$

which, since y_1 is already determined by the constraint, (6.16), is minimized by putting

$$y_2 = C_2^{-1} c_2.$$

Thus, we get an explicit formula for the solution of (6.12) in terms of the GSVD:

$$x = X \begin{pmatrix} S^{-1} & 0 \\ 0 & C_2^{-1} \end{pmatrix} \begin{pmatrix} V^T & 0 \\ 0 & U_2^T \end{pmatrix} \begin{pmatrix} d \\ c \end{pmatrix}.$$

6.9 Computing the SVD

The SVD is computed in MATLAB by the statement `[U,S,V]=svd(A)`. This statement is an implementation of algorithms from LAPACK [1] (the double precision high level driver algorithm for SVD is called `DGESVD`). In the algorithm the matrix is first reduced to bidiagonal form by a series of Householder transformation from the left and right. Then the bidiagonal matrix is iteratively reduced to diagonal form using a variant of the QR algorithm, see Chapter 16.

The SVD of a dense (full) matrix can be computed in $\mathcal{O}(mn^2)$ flops. The constant is usually $5 - 10$. For comparison we give flop counts for a few other matrix decompositions in Table 6.1.

The computation of a partial SVD of a large, sparse matrix is done in MATLAB by the statement `[U,S,V]=svds(A,k)`. This statement is based on Lanczos algorithms from ARPACK. We give a brief description of Lanczos algorithms in Chapter 16. For a more comprehensive treatment, see [4].