II.6 Singular Value Decomposition

In this chapter we discuss the *Singular Value Decomposition (SVD)*: a matrix factorisation that encodes how much a matrix "stretches" a random vector. This includes *singular values*, the largest of which dictates the 2-norm of the matrix.

Definition 1 (singular value decomposition) For $A \in \mathbb{C}^{m \times n}$ with rank r > 0, the *(reduced) singular value decomposition (SVD)* is

$$A = U\Sigma V^{\star}$$

where $U\in\mathbb{C}^{m\times r}$ and $V\in\mathbb{C}^{r\times n}$ have orthonormal columns and $\Sigma\in\mathbb{R}^{r\times r}$ is diagonal whose diagonal entries, which which we call *singular values*, are all positive and non-increasing: $\sigma_1\geq\cdots\geq\sigma_r>0$. The *full singular value decomposition (SVD)* is

$$A = U\Sigma V^{\star}$$

where $U\in U(m)$ and $V\in U(n)$ are unitary matrices and $\Sigma\in\mathbb{R}^{m\times n}$ has only diagonal non-zero entries, i.e., if m>n,

and if m < n,

$$\Sigma = egin{bmatrix} \sigma_1 & & & & & \ & \ddots & & & & \ & & \sigma_m & 0 & \cdots & 0 \end{bmatrix}$$

where $\sigma_k = 0$ if k > r.

In particular, we discuss:

- 1. Existence of the SVD: we show that an SVD exists by relating it to the eigenvalue Decomposition of $A^{\star}A$ and AA^{\star} .
- 2. 2-norm and SVD: the 2-norm of a matrix is defined in terms of the largest singular value.
- 3. Best rank-k approximation and compression: the best approximation of a matrix by a smaller rank matrix can be constructed

using the SVD, which gives an effective way to compress matrices.

In [1]: using LinearAlgebra, Plots

[Info: Precompiling Plots [91a5bcdd-55d7-5caf-9e0b-520d859cae80]

1. Existence

To show the SVD exists we first establish some properties of a *Gram matrix* (A^*A):

Proposition 1 (Gram matrix kernel) The kernel of A is the also the kernel of A^*A .

Proof If $A^{\star}A\mathbf{x}=0$ then we have

$$0 = \mathbf{x}^{\star} A^{\star} A \mathbf{x} = \|A \mathbf{x}\|^2$$

which means $A\mathbf{x}=0$ and $\mathbf{x}\in\ker(A)$.

Proposition 2 (Gram matrix diagonalisation) The Gram-matrix satisfies

$$A^{\star}A = Q\Lambda Q^{\star} \in \mathbb{C}^{n imes n}$$

is a Hermitian matrix where $Q\in U(n)$ and the eigenvalues λ_k are real and non-negative. If $A\in\mathbb{R}^{m\times n}$ then $Q\in O(n)$.

Proof A^*A is Hermitian so we appeal to the spectral theorem for the existence of the decomposition, and the fact that the eigenvalues are real. For the corresponding (orthonormal) eigenvector \mathbf{q}_k ,

$$\lambda_k = \lambda_k \mathbf{q}_k^\star \mathbf{q}_k = \mathbf{q}_k^\star A^\star A \mathbf{q}_k = \|A \mathbf{q}_k\|^2 \geq 0.$$

This connection allows us to prove existence:

Theorem 1 (SVD existence) Every $A \in \mathbb{C}^{m \times n}$ has an SVD.

Proof Consider

$$A^{\star}A = Q\Lambda Q^{\star}.$$

Assume (as usual) that the eigenvalues are sorted in decreasing modulus, and so $\lambda_1, \ldots, \lambda_r$ are an enumeration of the non-zero eigenvalues and

$$V:=[\,\mathbf{q}_1|\cdots|\mathbf{q}_r\,]$$

the corresponding (orthonormal) eigenvectors, with

$$K = ig[\mathbf{q}_{r+1} | \cdots | \mathbf{q}_n ig]$$

the corresponding kernel. Define

$$\Sigma := \left[egin{array}{ccc} \sqrt{\lambda_1} & & & \ & \ddots & & \ & & \sqrt{\lambda_r} \end{array}
ight]$$

Now define

$$U := AV\Sigma^{-1}$$

which is orthogonal since $A^{\star}AV=V\Sigma^2$:

$$U^{\star}U = \Sigma^{-1}V^{\star}A^{\star}AV\Sigma^{-1} = I.$$

Thus we have

$$U\Sigma V^\star = AVV^\star = A\underbrace{[\,V|K\,]}_Q\underbrace{\left[\!\!\begin{array}{c} V^\star \\ K^\star \end{array}\!\!\right]}_{Q^\star}$$

where we use the fact that AK=0 so that concatenating K does not change the value.

2. 2-norm and SVD

Singular values tell us the 2-norm:

Corollary 1 (singular values and norm)

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

and if $A \in \mathbb{C}^{n imes n}$ is invertible, then

$$\|A^{-1}\|_2 = \sigma_n^{-1}$$

Proof

First we establish the upper-bound:

$$||A||_2 \le ||U||_2 ||\Sigma||_2 ||V^{\star}||_2 = ||\Sigma||_2 = \sigma_1$$

This is attained using the first right singular vector:

$$\|A\mathbf{v}_1\|_2 = \|\Sigma V^\star \mathbf{v}_1\|_2 = \|\Sigma \mathbf{e}_1\|_2 = \sigma_1$$

The inverse result follows since the inverse has SVD

$$A^{-1} = V\Sigma^{-1}U^{\star} = (VW)(W\Sigma^{-1}W)(WU)^{\star}$$

is the SVD of A^{-1} , i.e. $VW \in U(n)$ are the left singular vectors and WU are the right singular vectors, where

$$W:=P_{\sigma}=\left[egin{array}{ccc} & 1\ dots & \ 1 \end{array}
ight]$$

is the permutation that reverses the entries, that is, σ has Cauchy notation

$$\begin{pmatrix} 1 & 2 & \cdots & n \\ n & n-1 & \cdots & 1 \end{pmatrix}.$$

We will not discuss in this module computation of singular value decompositions or eigenvalues: they involve iterative algorithms (actually built on a sequence of QR decompositions).

3. Best rank-k approximation and compression

One of the main usages for SVDs is low-rank approximation:

Theorem 2 (best low rank approximation) The matrix

$$A_k := \left[egin{array}{cccc} \mathbf{u}_1 | \cdots | \mathbf{u}_k \end{array}
ight] \left[egin{array}{cccc} \sigma_1 & & & \ & \ddots & & \ & & \sigma_k \end{array}
ight] \left[old \mathbf{v}_1 | \cdots | old \mathbf{v}_k \end{array}
ight]^\star$$

is the best 2-norm approximation of A by a rank k matrix, that is, for all rank-k matrices B, we have

$$||A - A_k||_2 \le ||A - B||_2$$

Proof We have

Suppose a rank-k matrix B has

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

For all $\mathbf{w} \in \ker(B)$ we have

$$||A\mathbf{w}||_2 = ||(A - B)\mathbf{w}||_2 \le ||A - B|| ||\mathbf{w}||_2 < \sigma_{k+1} ||\mathbf{w}||_2$$

But for all $\mathbf{u} \in \mathrm{span}(\mathbf{v}_1,\ldots,\mathbf{v}_{k+1})$, that is, $\mathbf{u} = V[:,1:k+1]\mathbf{c}$ for some $\mathbf{c} \in \mathbb{R}^{k+1}$ we have

$$\|A\mathbf{u}\|_2^2 = \|U\Sigma_k\mathbf{c}\|_2^2 = \|\Sigma_k\mathbf{c}\|_2^2 = \sum_{j=1}^{k+1} (\sigma_jc_j)^2 \geq \sigma_{k+1}^2\|c\|^2,$$

i.e., $||A\mathbf{u}||_2 \ge \sigma_{k+1}||c||$. Thus \mathbf{w} cannot be in this span.

The dimension of the span of $\ker(B)$ is at least n-k, but the dimension of $\operatorname{span}(\mathbf{v}_1,\ldots,\mathbf{v}_{k+1})$ is at least k+1. Since these two spaces cannot intersect (apart from at 0) we have a contradiction, since (n-r)+(r+1)=n+1>n.

Example 1 (Hilbert matrix) Here we show an example of a simple low-rank approximation using the SVD. Consider the Hilbert matrix:

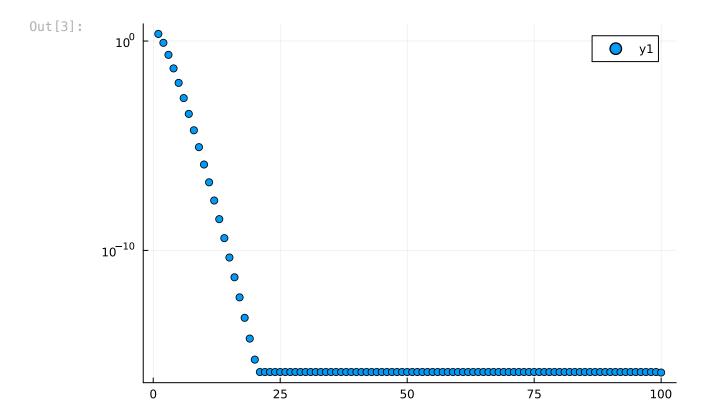
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In [2]: hilbertmatrix(n) = [1/(k+j-1) \text{ for } j = 1:n, k=1:n]
hilbertmatrix(5)
```

Out[2]: 5×5 Matrix{Float64}:

```
1.0
         0.5
                  0.333333 0.25
                                     0.2
0.5
         0.333333 0.25
                            0.2
                                     0.166667
0.333333 0.25
                  0.2
                            0.166667 0.142857
0.25
                  0.166667 0.142857
                                     0.125
         0.166667 0.142857 0.125
                                     0.111111
0.2
```

That is, the H[k,j]=1/(k+j-1). This is a famous example of matrix with rapidly decreasing singular values:

```
In [3]: H = hilbertmatrix(100)
U,σ,V = svd(H)
scatter(σ; yscale=:log10)
```



Note numerically we typically do not get a exactly zero singular values so the rank is always treated as $\min(m,n)$. Because the singular values decay rapidly we can approximate the matrix very well with a rank 20 matrix:

Out[4]: 8.20222266307798e-16

Note that this can be viewed as a *compression* algorithm: we have replaced a matrix with $100^2=10,000$ entries by two matrices and a vector with 4,000 entries without losing any information. In the problem sheet we explore the usage of low rank approximation to smooth functions and to compress images.