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Matrix Singular Value Decomposition

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MATRIX SINGULAR VALUE DECOMPOSITION

by

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Abstract

This thesis starts with the fundamentals of matrix theory and ends with applications of the matrix singular value decomposition (SVD). The background matrix theory coverage includes unitary and Hermitian matrices, and matrix norms and how they relate to matrix SVD. The matrix condition number is discussed in relationship to the solution of linear equations. Some inequalities based on the trace of a matrix, polar matrix decomposition, unitaries and partial isometies are discussed. Among the SVD applications discussed are the method of least squares and image compression. Expansion of a matrix as a linear combination of rank one partial isometries is applied to image compression by using reduced rank matrix approximations to represent greyscale images. MATLAB results for approximations of JPEG and .bmp images are presented. The results indicate that images can be represented with reasonable resolution using low rank matrix SVD approximations.

1 Introduction

The singular value decomposition (SVD) of a matrix is similar to the diagonalization of a normal matrix. Diagonalization of a matrix decomposes the matrix into factors using the eigenvalues and eigenvectors. Diagonalization of a matrix A is of the form $A = VDV^*$, where the columns of V are eigenvectors of A and form an orthonormal basis for $\mathbb{R}^n$ or $\mathbb{C}^n$, and D is a diagonal matrix with the diagonal elements consisting of the eigenvalues. On the other hand, the SVD factorization is of the form $A = U\Sigma V^*$. The columns of U and V are called left and right 'singular' vectors for A, and the matrix Σ is a diagonal matrix with diagonal elements consisting of the 'singular' values of A. The SVD is important and has many applications. Unitary matrices are analogous to phase factors and the singular values matrix is similar to the magnitude part of a polar decomposition of a complex number.

2 Background matrix theory

A matrix $A \in M_{m,n}(\mathbb{C})$ denotes an $m \times n$ matrix A with complex entries. Similarly $A \in M_n(\mathbb{C})$ denotes an $n \times n$ matrix with complex entries. The complex field ($\mathbb{C}$) will be assumed. In cases where real numbers apply, the real field ($\mathbb{R}$) will be specified. When the real field is considered, unitary matrices are replaced with real orthogonal matrices. We will often abbreviate $M_{m,n}(\mathbb{C})$, $M_n(\mathbb{C})$ to $M_{m,n}$ and M_n, respectively.

We remind the reader of a few basic definitions and facts.

Definition 1. *The* ***Hermitian adjoint*** *or* ***adjoint*** A^* *of* $A \in M_{m,n}$ *is defined by* $A^* = \bar{A}^T$, *where* $\bar{A}$ *is the component-wise conjugate, and* T *denotes the transpose. A matrix is* ***self-adjoint or Hermitian*** *if* $A^* = A$.

Definition 2. *A matrix* $B \in M_n$ *such that* $\langle Bx, x\rangle \geq 0$ *for all* $x \in \mathbb{C}^n$ *is said to be positive semidefinite; an equivalent condition is that* B *be Hermitian and have all eigenvalues nonnegative.*

Proposition 1. *Let* A *be a self-adjoint (Hermitian) matrix. Then every eigenvalue of* A *is real.*

Proof. Let λ be an eigenvalue and let x be a corresponding eigenvector. Then

$$\lambda \langle x, x\rangle = \langle \lambda x, x\rangle = \langle Ax, x\rangle$$

$$= \langle x, A^*x\rangle = \langle x, Ax\rangle = \langle x, \lambda x\rangle = \bar{\lambda} \langle x, x\rangle ,$$

$$\lambda x = A(x) = A^*(x) = \bar{\lambda}x.$$

Thus $\lambda = \bar{\lambda}$. So, the eigenvalue λ is real. $\square$

Definition 3. *A matrix* $U \in M_n$ *is said to be* ***unitary*** *if* $U^*U = UU^* = I_n$, *with* I_n *the* $n \times n$ *identity matrix. If* $U \in M_n(\mathbb{R})$, U *is* ***real orthogonal****.*

Definition 4. *A matrix* $A \in M_n$ *is* ***normal*** *if* $A^*A = AA^*$, *that is if* A *commutes with its Hermitian adjoint.*

Both the transpose and the Hermitian adjoint obey the *reverse-order law*: $(AB)^* = B^*A^*$ and $(AB)^T = B^TA^T$, if the products are defined. For the conjugate of a product, there is no reversing: $\overline{AB} = \bar{A}\bar{B}$.

Proposition 2. *Let a matrix $U \in M_n$ be unitary. Then (a) U^T, (b) U^*, (c) $\bar{U}$ are all unitary.*

Proof. (a) Given $UU^* = U^*U = I_n$, then U^T times the Hermitian conjugate of U^T is as follows:

$$U^T(U^T)^* = U^T\bar{U} = (U^*U)^T = (I_n)^T = I_n,$$

and since it results in an identity matrix I_n, then U^T is unitary, given U is unitary. Similarly,

$$U^*(U^*)^* = U^*U = I_n$$

and

$$\bar{U}(\bar{U})^* = \bar{U}U^T = \overline{UU^*} = \bar{I_n} = I_n.$$

□

Proposition 3. *The eigenvalues of the inverse of a matrix are the reciprocals of the matrix eigenvalues.*

Proof. Let λ be an eigenvalue of an invertible matrix A and let x be an eigenvector. Then

$$Ax = \lambda x,$$

so that

$$A^{-1}(\lambda x) = x$$

by the definition of a matrix inverse. Then

$$\lambda A^{-1}x = x$$

and

$$A^{-1}x = \frac{1}{\lambda}x.$$

□

Definition 5. *A matrix $B \in M_n$ is said to be **similar** to a matrix $A \in M_n$ if there exists a nonsingular matrix $S \in M_n$ such that $B = S^{-1}AS$. If S is unitary then A and B are **unitarily similar**.*

Theorem 1. *Let $A \in M_n(\mathbb{C})$. Then AA^* and A^*A are self-adjoint, and have the same eigenvalues (including multiplicity).*

Proof. We have

$$(AA^*)^* = ((A^*)^*A^*) = AA^*,$$

and so AA^* is self-adjoint. Similarly,

$$(A^*A)^* = A^*(A^*)^* = A^*A,$$

and so A^*A is also self-adjoint.

Let λ be an eigenvalue of AA^* with eigenspace E_λ. For $v \in E_\lambda$, we have

$$AA^*v = \lambda v.$$

Premultiplying by A^* leads to

$$A^*AA^*v = A^*\lambda v = \lambda A^*v.$$

Thus, A^*v is an eigenvector of A^*A with eigenvalue λ since

$$A^*A(A^*v) = \lambda(A^*v).$$

Moreover, for $\lambda \neq 0$, the map which sends eigenvector v of AA^* to eigenvector A^*v of A^*A is one-to-one. This is because if $v, w \in E_\lambda$ with $A^*v = A^*w$

$$AA^*v = AA^*w,$$

then

$$\lambda v = \lambda w$$

$$v = w.$$

Similarly, any eigenvalue of A^*A is an eigenvalue of AA^* with eigenvector Av such that the corresponding map from the eigenspace E_λ of A^*A is one-to-one, for $\lambda \neq 0$.

Thus, for any non-zero eigenvalue λ of A^*A and AA^*, their corresponding eigenspaces have the same dimension. Since A^*A and AA^* are self-adjoint and have the same dimensions, it follows that the eigenspaces corresponding to an eigenvalue of zero also have the same dimension. Thus the multiplicities of a zero eigenvalue are the same, as well.

□

Corollary 1. *The matrices AA^* and A^*A are unitarily similar.*

Proof. Since A^*A and AA^* have the same eigenvalues and are both self-adjoint, they are unitarily diagonizable as follows:

$$AA^* = U^* \begin{bmatrix} \lambda_1 & & \\ & \ddots & \\ & & \lambda_n \end{bmatrix} U$$

and

$$A^*A = V^* \begin{bmatrix} \lambda_1 & & \\ & \ddots & \\ & & \lambda_n \end{bmatrix} V$$

with the same eigenvalues and possibly different unitary matrices U and V. Then

$$UAA^*U^* = \begin{bmatrix} \lambda_1 & & \\ & \ddots & \\ & & \lambda_n \end{bmatrix} = VA^*AV^*.$$

Thus,

$$AA^* = U^*VA^*AV^*U,$$

where U^*V and V^*U are unitary matrices. □

Lemma 1. *Suppose that H, K are positive semidefinite and that $H^2 = K^2$, where H^2 and K^2 are also positive semidefinite. Then $H = K$.*

Proof. Let U be a unitary matrix and D a diagonal matrix such that

$$H^2 = U^* D U.$$

Let $\sqrt{D}$ denote the matrix obtained from D by taking the entry-wise square root. Let

$$A = U^* \sqrt{D} U.$$

Then

$$A^2 = U^* \sqrt{D} U U^* \sqrt{D} U = U^* D U = H^2.$$

To prove the result, it suffices to show $H = A$. Let $d_1, \ldots, d_n$ be the diagonal entries of D. Then there is a polynomial P such that

$$P(d_i) = \sqrt{d_i}$$

for $i = 1, \ldots, n$. (The polynomial P may be obtained from the Lagrange Interpolation Formula.) Then

$$P(H^2) = P(U^* D U) = U^* P(D) U = U^* \sqrt{D} U = A.$$

Thus

$$HA = HP(H^2) = P(H^2)H = AH.$$

Thus H and A commute and both are positive semidefinite. It follows that they are simultaneously diagonalizable. Thus there exists a unitary V and diagonal matrices D_1 and D_2 such that $H = V^* D_1 V$ and $A = V^* D_2 V$. Also, since $H^2 = A^2$, we have

$$V^* D_1^2 V = V^* D_2^2 V,$$

$$D_1^2 = D_2^2,$$

$$D_1 = D_2,$$

and so

$$H = A.$$

□

Definition 6. *The* ***Euclidean norm*** *(or* ℓ_2***-norm****) on* $\mathbb{C}^n$ *is*

$$\|x\|_2 \equiv (|x_1|^2 + \cdots + |x_n|^2)^{\frac{1}{2}}.$$

Moreover, $\|x - y\|_2$ measures the standard Euclidean distance between two points $x, y \in \mathbb{C}^n$. This is also derivable from the Euclidean inner product; that is

$$\|x\|_2^2 = \langle x, x \rangle = x^* x.$$

We call a function $\|\bullet\| : M_n \to \mathbb{R}$ a matrix norm if for all $A, B \in M_n$ it satisfies the following:

1. $\|A\| \geq 0$
2. $\|A\| = 0 \text{ iff } A = 0$
3. $\|cA\| = |c| \, \|A\|$ for all complex scalars c
4. $\|A + B\| \leq \|A\| + \|B\|$
5. $\|AB\| \leq \|A\| \, \|B\|$.

Definition 7. *Let* A *be a complex (or real)* $m \times n$ *matrix. Define the* ***operator norm****, also known as the* ***least upper bound norm (lub norm)****, of* A *by*

$$\|A\| \equiv \max \left(\frac{\|Ax\|}{\|x\|} \right) \quad x \neq 0.$$

We assume $x \in \mathbb{C}^n$ *or* $x \in \mathbb{R}^n$*. We will use the* $\| \ \|$ *notation to refer to a generic matrix norm or the operator norm depending on the context.*

Definition 8. *The* ***matrix Euclidean norm*** $\|\bullet\|_2$ *is defined on* M_n *by*

$$\|A\|_2 \equiv \left(\sum_{i,j=1}^{n} |a_{ij}|^2 \right)^{\frac{1}{2}}.$$

This matrix norm defined above is sometimes called the **Frobenius norm, Schur norm**, or the **Hilbert-Schmidt norm**. If, for example, $A \in M_n$ is written in terms of its column vectors $a_i \in \mathbb{C}^n$, then

$$\|A\|_2^2 = \|a_1\|_2^2 + \cdots + \|a_n\|_2^2 .$$

Definition 9. *The **spectral norm** is defined on M_n by*

$$|||A|||_2 \equiv \max\{\sqrt{\lambda} : \quad \lambda\, is\, an\, eigenvalue\, of\; A^*A.\}$$

Each of these norms on M_n is a matrix norm as defined above.

Definition 10. *Given any matrix norm $\|\ \|$, the matrix **condition number** of A, cond(A), is defined as*

$$cond(A) \equiv \begin{cases} \left\|A^{-1}\right\| \|A\|, & \textit{if } A \textit{ is nonsingular;} \\ \infty, & \textit{if } A \textit{ is singular.} \end{cases}$$

Usually $\|\bullet\|$ will be the lub-norm.

In mathematics, computer science, and related fields, *big O* notation (also known as *Big Oh* notation, Landau notation, Bachmann–Landau notation, and asymptotic notation) describes the limiting behavior of a function when the argument tends towards a particular value or infinity, usually in terms of simpler functions.

Definition 11. *Let $f(x)$ and $g(x)$ be two functions defined on some subset of the real numbers. One writes*

$$f(x) = O(g(x)) \text{ as } x \to \infty$$

if and only if, for sufficiently large values of x, $f(x)$ is at most a constant times $g(x)$ in absolute value. That is, $f(x) = O(g(x))$ if and only if there exists a positive real number M and a real number x_0 such that

$$|f(x)| \leq M|g(x)| \text{ for all } x > x_0.$$

Big O notation allows its users to simplify functions in order to concentrate on their growth rates: different functions with the same growth rate may be represented using the same O notation.

3 The singular value decomposition

3.1 Existence of the singular value decomposition

For convenience, we will often work with linear transformations instead of with matrices directly. Of course, any of the following results for linear transformations also hold for matrices.

Theorem 2 (Singular Value Theorem [2]). *Let V and W be finite-dimensional inner product spaces, and let $T : V \to W$ be a linear transformation of rank r. Then there exist orthonormal bases $\{v_1, v_2, \cdots, v_n\}$ for V and $\{u_1, u_2, \cdots, u_m\}$ for W and positive scalars $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_r$ such that*

$$T(v_i) = \begin{cases} \sigma_i u_i & \text{if } 1 \leq i \leq r \\ 0 & \text{if } i > r. \end{cases}$$

Conversely, suppose that the preceding conditions are satisfied. Then for $1 \leq i \leq n$, v_i is an eigenvector of T^*T with corresponding eigenvalue of σ_i^2 if $1 \leq i \leq r$ and 0 if $i > r$. Therefore the scalars $\sigma_1, \sigma_2, \cdots, \sigma_r$ are uniquely determined by T.

Proof. A basic result of linear algebra says that rank T = rank T^*T. Since T^*T is a positive semidefinite linear operator of rank r on V, there is an orthonormal basis $\{v_1, v_2, \cdots, v_n\}$ for V consisting of eigenvectors of T^*T with corresponding eigenvalues λ_i, where $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_r > 0$, and $\lambda_i = 0$ for $i > r$. For $1 \leq i \leq r$, define $\sigma_i = \sqrt{\lambda_i}$ and

$$u_i = \frac{1}{\sigma_i} T(v_i).$$

Suppose $1 \leq i, j \leq r$. Then

$$\langle u_i, u_j \rangle = \left\langle \frac{1}{\sigma_i} T(v_i), \frac{1}{\sigma_j} T(v_j) \right\rangle = \frac{1}{\sigma_i \sigma_j} \langle \lambda_i v_i, v_j \rangle = \frac{\sigma_i^2}{\sigma_i \sigma_j} \langle v_i, v_j \rangle = \delta_{ij},$$

where $\delta_{ij} = 1$ for $i = j$, and 0 otherwise. Hence, $\{u_1, u_2, \cdots, u_r\}$ is an orthonormal subset of W. This set can be extended to an orthonormal basis $\{u_1, u_2, \cdots, u_r, \cdots, u_m\}$ for W. Then $T(v_i) = \sigma_i v_i$ if $1 \leq i \leq r$, and $T(v_i) = 0$ if $i > r$.

Suppose that $\{v_1, v_2, \cdots, v_n\}$ and $\{u_1, u_2, \cdots, u_m\}$ and $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_r > 0$ satisfy the properties given in the first part of the theorem. Then for $1 \leq i \leq m$ and $1 \leq j \leq n$,

$$\langle T^*(u_i), v_j \rangle = \langle u_i, T(v_j) \rangle = \begin{cases} \sigma_i & \text{if } i = j \leq r \\ 0 & \text{otherwise} \end{cases}.$$

Thus,

$$T^*(u_i) = \sum_{j=1}^{n} \langle T^*(u_i), v_j \rangle \, v_j = \begin{cases} \sigma_i v_i & \text{if } i = j \leq r \\ 0 & \text{otherwise} \end{cases}.$$

For $i \leq r$,

$$T^*T(v_i) = T^*(\sigma_i u_i)) = \sigma_i T^*(u_i) = \sigma_i^2 u_i,$$

and for $i > r$

$$T^*T(v_i) = T^*(0) = 0.$$

Each v_i is an eigenvector of T^*T with eigenvalue σ_i^2 if $i \leq r$ and 0 if $i > r$. Thus the scalars σ_i are uniquely determined by T^*T.

$\square$

Definition 12. *The unique scalars $\sigma_1, \sigma_2, \cdots, \sigma_r$ in the theorem above (Theorem 2) are called the **singular values** of T. If r is less than both m and n, then the term singular value is extended to include $\sigma_{r+1} = \cdots = \sigma_k = 0$, where k is the minimum of m and n.*

Remark 1. *Thus for an $m \times n$ matrix A, by Theorem 2, the singular values of A are precisely the square roots of the the eigenvalues of A^*A.*

Theorem 3 (Singular Value Decomposition)**.** *If $A \in M_{m,n}$ has rank r with positive singular values $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_r$, then it may be written in the form*

$$A = V \Sigma W^*$$

where $V \in M_m$ and $W \in M_n$ are unitary and the matrix $\Sigma = [\Sigma_{ij}] \in M_{m,n}$ is given by

$$\Sigma_{ij} = \begin{cases} \sigma_i & \textit{if } i = j \leq r \\ 0 & \textit{otherwise} \end{cases}.$$

The proof of this is given in the proof Theorem 4, which contains this result.

Definition 13. *If $A \in M_{m,n}$ has rank r with positive singular values $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_r$, then a* ***singular value decomposition*** *of A is a factorization $A = U\Sigma W^*$, where U and W are unitary and Σ is the $m \times n$ matrix defined as in Theorem 3.*

Example 1.

$$A = \begin{bmatrix} i+1 & 1 \\ 1-i & -i \end{bmatrix},$$

$$A^*A = \begin{bmatrix} 4 & 2(1-i) \\ 2(1+i) & 2 \end{bmatrix}$$

The eigenvalues of A^*A are obtained from

$$det \begin{vmatrix} 4-\lambda & 2(i-1) \\ 2(i+1) & 2-\lambda \end{vmatrix} = 0,$$

leading to the characteristic polynomial

$$(4-\lambda)(2-\lambda) - 8 = 0.$$

Then $\lambda = 6$ and $\lambda = 0$ are the eigenvalues. The singular values are respectively $\sigma_1 = \sqrt{6}$ and $\sigma_2 = 0$. Thus

$$\Sigma = \begin{pmatrix} \sqrt{6} & 0 \\ 0 & 0 \end{pmatrix}.$$

A normalized eigenvector for the eigenvalue 6 is

$$\begin{pmatrix} \frac{2}{\sqrt{6}} \\ \frac{1+i}{\sqrt{6}} \end{pmatrix}.$$

Then

$$w_1 = \begin{pmatrix} \frac{2}{\sqrt{6}} \\ \frac{1+i}{\sqrt{6}} \end{pmatrix},$$

and a normalized eigenvector that corresponds to $\lambda_2 = 0$ is

$$w_2 = \begin{pmatrix} \frac{1-i}{\sqrt{6}} \\ \frac{-2}{\sqrt{6}} \end{pmatrix},$$

which leads to

$$W = \begin{pmatrix} \frac{2}{\sqrt{6}} & \frac{1-i}{\sqrt{6}} \\ \frac{1+i}{\sqrt{6}} & \frac{-2}{\sqrt{6}} \end{pmatrix}.$$

The columns of W span $\mathbb{C}^2$ and the matrix U is found as follows:

$$u_1 = \frac{1}{\sqrt{6}} A w_1 = \begin{pmatrix} \frac{1+i}{2} \\ \frac{1-i}{2} \end{pmatrix},$$

and

$$u_2 = \frac{1}{\sqrt{6}} A w_2 = \begin{pmatrix} \frac{1+i}{2} \\ \frac{-1+i}{2} \end{pmatrix}.$$

A singular value decomposition is then

$$A = \begin{pmatrix} \frac{1+i}{2} & \frac{1+i}{2} \\ \frac{1-i}{2} & \frac{-1+i}{2} \end{pmatrix} \begin{pmatrix} \sqrt{6} & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} \frac{2}{\sqrt{6}} & \frac{1-i}{\sqrt{6}} \\ \frac{1+i}{\sqrt{6}} & \frac{-2}{\sqrt{6}} \end{pmatrix}^*.$$

In the example above, the singular values are uniquely defined by A, but the orthonormal basis vectors which form the columns of the unitary matrices V and W are not uniquely determined as there is more than one orthonormal basis consisting of eigenvectors of A^*A.

Proposition 4. *Let $A = U\Sigma W^*$, where U and W are unitary and Σ is diagonal matrix with positive diagonal entries $\sigma_1, \ldots, \sigma_q$. Then $\sigma_1, \ldots, \sigma_q$ are the singular values of A and $U\Sigma W^*$ is a singular value decomposition of A.*

Proof. Let $A = U\Sigma W^*$. Then

$$A^*A = W\Sigma^*\Sigma W^*.$$

Then $\Sigma^*\Sigma$ is diagonal with diagonal entries $\sigma_1^2, \sigma_2^2, \ldots, \sigma_q^2$, which are the eigenvalues of A^*A. Therefore, the singular values of A are $\sigma_1, \sigma_2, \ldots, \sigma_q$. □

Most treatments of the existence of the SVD follow the argument in the example above. Below are the details of the first proof sketched out by Autonne [1]. We use matrix diagonalization below as a means to perform singular value decomposition for a square matrix $A \in M_n(\mathbb{C})$ and extend this to an $m \times n$ matrix.

Theorem 4. *Let $A \in M_n(\mathbb{C})$ and let $U \in M_n(\mathbb{C})$ be unitary such that*

$$A^*A = U(AA^*)U^*.$$

Then,

(a.) UA is normal and

$$A = V\Sigma W^*,$$

where V and W are unitary matrices, and Σ is the diagonal matrix consisting of the singular values of A along the diagonal.

(b.) This can be extended to $A \in M_{m,n}(\mathbb{C})$

Proof. (a.)

$$(UA)(UA)^* = (UA)A^*U^* = A^*A$$

and

$$(UA)^*(UA) = A^*U^*UA = A^*A.$$

Since UA is normal it is diagonalizable. Thus, there is a unitary $X \in M_n$ and a diagonal matrix $\Lambda \in M_n$ such that $UA = X\Lambda X^*$. Using the polar form of a complex number $\lambda = |\lambda| e^{i\theta}$, we can write $\Lambda = \Sigma D$, where $\Sigma = |\Lambda|$ has nonnegative entries ($|\Lambda|$ is the matrix consisting of the entrywise absolute values $[|a_{ij}|]$ of the matrix Λ) and D is a diagonal unitary matrix. Explicitly,

$$\Lambda = \begin{bmatrix} \lambda_1 & & & \\ & \lambda_2 & & \\ & & \ddots & \\ & & & \lambda_n \end{bmatrix} = \begin{bmatrix} |\lambda_1| & & & \\ & |\lambda_2| & & \\ & & \ddots & \\ & & & |\lambda_n| \end{bmatrix} \begin{bmatrix} e^{i\theta_1} & & & \\ & e^{i\theta_2} & & \\ & & \ddots & \\ & & & e^{i\theta_n} \end{bmatrix}.$$

The first matrix is identified as Λ, the second as Σ, and the third as D making up $\Lambda = \Sigma D$. With $UA = X\Lambda X^*$ and $\Lambda = \Sigma D$, this leads to

$$UA = X\Sigma D X^*.$$

Left multiplying by U^* results in:

$$U^*UA = U^*X\Sigma D X^*$$

and

$$A = V\Sigma W^*$$

with $V = U^*X$, and $W = XD^*$.

(b.) If $A \in M_{m,n}$ with $m > n$, let $u_1, \cdots, u_\nu$ be an orthonormal basis for the null space $N(A^*) \subseteq \mathbb{C}^m$ of A^*. The matrix $A^* \in M_{n,m}$ and nullity A^* + rank $A^* = m$. So the nullity ν of A^* satisfies

$$\nu = m - \operatorname{rank} A^* \geq m - n,$$

since rank $A^* \leq n$. Let $U_2 = [u_1 \cdots u_{m-n}] \in M_{m,m-n}$. Extend $\{u_1, \cdots, u_{m-n}\}$ to a basis of $\mathbb{C}^m$:

$$B = \{u_1, \cdots, u_{m-n}, w_1, \cdots, w_n\}.$$

Let $U_1 = [w_1 \cdots w_n]$ and let $U = [U_1 \quad U_2] \in M_m$ which is unitary. Then

$$A^*U = A^*[U_1 \quad U_2] = [A^*U_1 \quad A^*U_2] = [0 \quad A^*U_2]$$

and so

$$U^*A = \begin{bmatrix} A_1 \\ 0 \end{bmatrix},$$

where $A_1 = U_2^*A$, with $A_1 \in M_n$. By the previous part, there are unitaries V and W and a diagonal matrix Σ such that

$$A_1 = V\Sigma W^*.$$

Then

$$A = U \begin{bmatrix} A_1 \\ 0 \end{bmatrix} = U \begin{bmatrix} V\Sigma W^* \\ 0 \end{bmatrix} = U \begin{bmatrix} V & 0 \\ 0 & I \end{bmatrix} \begin{bmatrix} \Sigma \\ 0 \end{bmatrix} W^*.$$

Let

$$\tilde{U} \equiv U \begin{bmatrix} V & 0 \\ 0 & I \end{bmatrix}$$

and

$$\tilde{\Sigma} \equiv \begin{bmatrix} \Sigma \\ 0 \end{bmatrix}.$$

This leads to the singular value decomposition

$$A = \tilde{U}\tilde{\Sigma}W^*.$$

If $A \in M_{m,n}$ and $n > m$, then $A^* \in M_{n,m}$, the argument above applies to $A^* \in M_{n,m}$, to get $A^* = V\Sigma W^*$, and so $A = W\Sigma V^*$.

□

3.2 Basic properties of singular values and the SVD

Proposition 5. *For a matrix $A \in M_{m,n}$ the rank of A is exactly the same as the number of its nonzero singular values.*

Proof. Let $A = V\Sigma W^*$ be the SVD with V, W unitary. Since V and W are unitary matrices, multiplication by V and W (which is equivalent to elementary row and column operations) does not change the rank of a matrix.

As a result rank A= rank AW = rank $V\Sigma$ =rank Σ, which is exactly the number of the nonzero singular values.

□

Remark 2. *Suppose $A \in M_n$ is normal, the spectral decomposition*

$$A = U\Lambda U^*$$

with unitary $U \in M_n$,

$$\Lambda = diag\left(\lambda_1, \cdots, \lambda_n\right),$$

and

$$|\lambda_1| \geq \cdots \geq |\lambda_n| \,.$$

If we let

$$\Sigma \equiv diag(|\lambda_1|\,, \cdots, |\lambda_n|)$$

then $\Lambda = D\Sigma$, *where*

$$D = diag(e^{i\theta_1}, \cdots, e^{i\theta_n})$$

is a diagonal matrix. Thus

$$A = U\Lambda U^* = (UD)\Sigma U^* = V\Sigma W^*,$$

which is a singular value decomposition of A *with* $V = UD$ *and* $W = U$. *The singular values are just the absolute values of the eigenvalues for a normal matrix.*

Proposition 6. *The singular values of* U_1AU_2 *are the same as those of* A *whenever* U_1 *and* U_2 *are unitary matrices.*

Proof. Let $B = U_1AU_2$. Then,

$$B^*B = (U_1AU_2)^*(U_1AU_2) = (U_2^*A^*U_1^*U_1AU_2) = U_2^*A^*AU_2.$$

Thus, B^*B and A^*A are unitarily similar, with $U_2^* = U_2^{-1}$ since U_2 is unitary. By similarity, B^*B and A^*A have the same eigenvalues, and so by Theorem 2 and the definition of singular value, A and B have the same singular values. □

We note again that the nonzero singular values of $A = V\Sigma W^*$ are exactly the nonnegative square roots of the nonzero eigenvalues of either

$$A^*A = W\Sigma^T\Sigma W^* \quad or \quad AA^* = V\Sigma\Sigma^T V^*.$$

Consequently the ordered singular values of A are uniquely determined by A, and they are the same as the singular values of A^*. The singular values of U_1AU_2 are the same as those of A, whenever U_1 and U_2 are unitary matrices that respectively left multiply and right multiply into A. There is therefore, unitary invariance of the set of singular values of a matrix.

Theorem 5. *Let $A \in M_{m,n}$ and $A = V\Sigma W^*$, a singular value decomposition of A. Then the singular values of A^*, A^T, $\bar{A}$ are all the same, and if $m = n$ and A is nonsingular, the singular values of A are the reciprocals of the singular values of A^{-1}.*

Proof. First,

$$A^* = (V\Sigma W^*)^* = (W^*)^*\Sigma^* V^* = W\Sigma^* V^*,$$

which shows A^* and A have the same singular values since the entries of Σ are real. This is the same singular value decomposition except for W taking the role of V since if $A \in M_{m,n}$, $A^* \in M_{n,m}$, and Σ^* has the same nonzero singular values as Σ. Similarly,

$$A^T = (V\Sigma W^*)^T = (W^*)^T \Sigma^T V^T.$$

Since Σ^T has the same nonzero entries as Σ, it follows that A and A^T have the same singular values. For $\bar{A}$, we have

$$\bar{A} = \bar{V}\bar{\Sigma}\bar{W}^*.$$

Since Σ is a real matrix, $\bar{\Sigma} = \Sigma$, and so A and $\bar{A}$ have the same singular values. For A^{-1}, we have

$$A^{-1} = (W^*)^{-1}\Sigma^{-1}V^{-1} = W\Sigma^{-1}V^*$$

since V and W are unitary. Then

$$A^{-1} = (W^*)^{-1}\Sigma^{-1}V^{-1} = W\Sigma^{-1}V^* = W \begin{bmatrix} \frac{1}{\sigma_1} & & \\ & \ddots & \\ & & \frac{1}{\sigma_n} \end{bmatrix} V^*.$$

Hence, the singular values of A^{-1} are $\frac{1}{\sigma_1}, \frac{1}{\sigma_2} \cdots, \frac{1}{\sigma_n}$. $\square$

Theorem 6. *The singular value decomposition of a vector $v \in \mathbb{C}^n$ (viewed as an $n \times 1$ matrix) is of the form:*

$$v = U\Sigma W^*$$

with U an $n \times n$ unitary matrix with the first column vector the same as the normalized given vector v,

$$\Sigma = \begin{bmatrix} \|v\| \\ 0 \\ \vdots \\ 0 \end{bmatrix},$$

and

$$W = [1].$$

Proof. For a vector $v \in \mathbb{C}^n$,

$$v^* v = \|v\|^2 .$$

The eigenvalues of v^*v are then obtained by

$$\|v\|^2 - \lambda = 0.$$

This leads to $\lambda = \|v\|^2$, and the singular value $\sigma = \sqrt{\|v\|^2} = \|v\|$. Extend $\left\{ \frac{v}{\|v\|} \right\}$ to an orthonormal basis $\left\{ \frac{v}{\|v\|}, w_2, w_3, \ldots, w_n \right\}$ of $\mathbb{C}^n$. Let U be the matrix whose columns are members of this basis with $\frac{v}{\|v\|}$ the first column. Let $W = [1]$ and

$$\Sigma = \begin{bmatrix} \|v\| \\ 0 \\ \vdots \\ 0 \end{bmatrix}.$$

Then the singular value decomposition of the vector v is given by

$$v = \begin{bmatrix} v & w_2 & \cdots & w_n \end{bmatrix} \begin{bmatrix} \|v\| \\ 0 \\ \vdots \\ 0 \end{bmatrix} \begin{bmatrix} 1 \end{bmatrix}.$$

□

Proposition 7. *A matrix $A \in M_n$ is unitary if and only if all the singular values ; σ_i of the matrix are equal to* 1 *for all $i = 1, \cdots, n$.*

Proof. ($\Rightarrow$) Assume $A \in M_n$ is unitary. Then $A^*A = I_n$ has all eigenvalues equal to 1. Hence, the singular values of A are equal to 1. ($\Leftarrow$)Let $A = U\Sigma W^*$ be a singular value decomposition. Assume $\sigma_i = 1$ for $1 \leq i \leq n$. Then

$$A = UI_nW^* = UW^*,$$

a product of unitary matrices. So A is unitary.

□

3.3 A geometric interpretation of the SVD

Suppose A is an $m \times n$ real matrix of rank k with singular values $\sigma_1, \ldots, \sigma_n$. Then there exist orthonormal bases $\{v_1, \ldots, v_n\}$ and $\{u_1, \ldots, u_m\}$ such that $Av_i = \sigma_i u_i$ for $1 \leq i \leq k$, and $Av_i = 0$ for $k < i \leq n$.

Now consider the unit ball in $\mathbb{R}^n$. An arbitrary element x of the unit ball can be represented by $x = x_1v_1 + x_2v_2 + \cdots + x_nv_n$, with $\sum_{i=1}^n x_i^2 \leq 1$. Thus, the image of x under A is

$$Ax = \sigma_1 x_1 u_1 + \ldots + \sigma_k x_k u_k.$$

So the image of the unit sphere consists of the vectors $y_1u_1 + y_2u_2 + \ldots + y_ku_k$, where $y_i = \sigma_i x_i$ and

$$\frac{y_1^2}{\sigma_1^2} + \frac{y_2^2}{\sigma_2^2} + \ldots + \frac{y_k^2}{\sigma_k^2} = \sum_{i=1}^{k} x_i^2 \leq 1.$$

Since $k \leq n$ this shows that A maps the unit sphere in $\mathbb{R}^n$ to a k-dimensional ellipsoid with semi-axes in the directions u_i, and with the magnitudes σ_i. The image of A first collapses $n - k$ dimensions of the domain, then distorts the remaining dimensions, stretching and squeezing the unit k-sphere into an ellipsoid, and finally it embeds the ellipsoid in $\mathbb{R}^m$.

3.4 Condition numbers, singular values and matrix norms

We next examine the relationship between singular values of a matrix, condition number and a matrix norm.

We start with some theorems that relate matrix condition numbers to matrix norms and singular values. We then later give an example of an ill conditioned A for which all the rows and columns have nearly the same norm. This affects computational stability when solving systems of equations as digital storage can vary depending on machine precision.

In solving a system of equations

$$Ax = b,$$

experimental errors and computer errors occur. There are systematic and random errors in the measurements to obtain data for the system of equations, and the computer representation of the data is subject to the limitations of the computer's digital precision. We would wish that small relative changes in the coefficients of the system of equations should cause small relative errors in the solution. A system that has this desirable property is called *well-conditioned*, otherwise it is *ill-conditioned*. As an example, the system

$$\begin{aligned} x_1 + x_2 &= 5 \\ x_1 + x_2 &= 1 \end{aligned} \tag{1}$$

has the solution

$$\begin{bmatrix} 3 \\ 2 \end{bmatrix}.$$

Changing

$$b = \begin{bmatrix} 5 \\ 1 \end{bmatrix}$$

by a small percent leads to

$$\begin{aligned} x_1 + x_2 &= 5 \\ x_1 + x_2 &= 1.0001. \end{aligned} \tag{2}$$

The change in b is

$$\delta b = \begin{bmatrix} 0 \\ 0.0001 \end{bmatrix}.$$

This has the solution

$$\begin{bmatrix} 3.00005 \\ 1.99995 \end{bmatrix}.$$

So this is an example of a well-conditioned system.

Define the *relative change* in b as

$$\frac{\|\delta b\|}{\|b\|}, \text{ where } \|b\| = \sqrt{\langle b, b\rangle}.$$

Definition 14. *Let B be an $n \times n$ self-adjoint matrix. The Rayleigh quotient for $x \neq 0$ is defined to be the scalar*

$$R(x) = \frac{\langle Bx, x\rangle}{\|x\|^2}.$$

Theorem 7. *For a self-adjoint matrix $B \in M_{n,n}$, $\max(R(x))$ is the largest eigenvalue of B and $\min(R(x))$ is the smallest eigenvalue of B.*

Proof. Choose an orthonormal basis $\{v_1, v_2, \cdots, v_n\}$ consisting of the eigenvectors of B such that $Bv_i = \lambda_i v_i$ $(1 \leq i \leq n)$ where $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$ are the eigenvalues of B. The eigenvalues of B are real since it is self-adjoint.

For $x \in \mathbb{C}^n$, there exists scalars $a_1, a_2, \cdots, a_n$ such that

$$x = \sum_{i=1}^{n} a_i v_i.$$

Therefore

$$R(x) = \frac{\langle Bx, x\rangle}{\|x\|^2} = \frac{\left\langle \sum_{i=1}^n a_i \lambda_i v_i, \sum_{j=1}^n a_j v_j \right\rangle}{\|x\|^2} = \frac{\sum_{i=1}^n \lambda_i |a_i|^2}{\|x\|^2} \leq \frac{\lambda_1 \sum_{i=1}^n |a_i|^2}{\|x\|^2} = \lambda_1.$$

It follows that $\max(R(x)) \leq \lambda_1$. Since $R(v_1) = \lambda_1$, $\max(R(x)) = \lambda_1$.

The second half of the theorem concerning the least eigenvalue follows by

$$R(x) = \frac{\sum_{i=1}^{n} \lambda_i |a_i|^2}{\|x\|^2} \geq \frac{\lambda_n \sum_{i=1}^{n} |a_i|^2}{\|x\|^2} = \lambda_n.$$

It follows that $\min R(x) \geq \lambda_n$. and since $R(v_n) = \lambda_n$, $\min R(x) = \lambda_n$. $\square$

Corollary 2. *For any square matrix A, $\|A\|$ (the* lub *norm)is finite and equals σ_1, the largest singular value of A.*

Proof. Let B be the self-adjoint matrix A^*A, and let λ be the largest eigenvalue of B. Assuming $x \neq 0$ then

$$0 \leq \frac{\|Ax\|^2}{\|x\|^2} = \frac{\langle Ax, Ax\rangle}{\|x\|^2} = \frac{\langle A^*Ax, x\rangle}{\|x\|^2} = \frac{\langle Bx, x\rangle}{\|x\|^2} = R(x).$$

Since

$$\|A\| = \max \frac{\|Ax\|}{\|x\|} \quad x \neq 0$$

$$\|A\|^2 = \max \frac{\|A\|^2}{\|x\|^2} = \max\ R(x) = \lambda$$

by Theorem 7. Then

$$\|A\| = \sqrt{\lambda}.$$

$\square$

Corollary 3. *Let A be an invertible matrix . Then*

$$\|A^{-1}\| = \frac{1}{\sigma_1(A)}.$$

Proof. For an invertible matrix, λ is an eigenvalue iff λ^{-1} is an eigenvalue of the inverse (Corollary 2). Let $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$ be the eigenvalues of A^*A. Then

$$\|A^{-1}\|^2$$

equals the square root of the largest eigenvalue of

$$A^{-1}(A^{-1})^* = (A^*A)^{-1}$$

and this is

$$\frac{1}{\lambda_n} = \frac{1}{\sigma_n(A)}.$$

$\square$

Theorem 8. *For the system $Ax = b$ where A is invertible and $b \neq 0$*

(a.)

$$\frac{1}{cond(A)} \frac{\|\delta b\|}{\|b\|} \leq \frac{\|\delta x\|}{\|x\|} \leq cond(A) \frac{\|\delta b\|}{\|b\|}.$$

(b.) If $\|\bullet\|$ is the operator norm, then

$$cond(A) = \sqrt{\frac{\lambda_1}{\lambda_n}} = \frac{\sigma_1(A)}{\sigma_n(A)}$$

where λ_1 and λ_n are the largest and smallest eigenvalues, respectively of A^*A.

Proof. Assuming A is invertible and $b \neq 0$ with $Ax = b$, for a given δb, let δx be the vector that satisfies

$$A(x + \delta x) = b + \delta b.$$

Since $Ax = b$ and $\delta x = A^{-1}(\delta b)$, we have

$$\|b\| = \|Ax\| \leq \|A\| \|x\|,$$

and

$$\|\delta x\| \leq \left\|A^{-1}\right\| \|\delta b\|.$$

Therefore,

$$\frac{\|\delta x\|}{\|x\|} \leq \frac{\|\delta x\|}{\|b\| / \|A\|} = \frac{\|A\| \|\delta x\|}{\|b\|} \leq \frac{\|A\| \left\|A^{-1}\right\| \|\delta b\|}{\|b\|} = \frac{\mathrm{cond}(A) \|\delta b\|}{\|b\|}.$$

Since $A^{-1}b = x$ and $\delta b = A(\delta x)$, we have

$$\|x\| \leq \left\|A^{-1}\right\| \|b\|$$

and

$$\|\delta b\| \leq \|A\| \|\delta x\|.$$

Therefore,

$$\frac{\|\delta x\|}{\|x\|} \geq \frac{\|\delta x\|}{\|A^{-1}\| \, \|b\|} \geq \frac{\|\delta b\|}{\|A^{-1}\| \, \|A\| \, \|b\|} = \frac{1}{\text{cond}(A)} \frac{\|\delta b\|}{\|b\|}.$$

Statement (a.) in the theorem above follows immediately from the inequalities above, and (b.) follows from the corollaries above and Theorem 7:

$$\text{cond(A)} = \sqrt{\frac{\lambda_1}{\lambda_n}}.$$

□

Corollary 4. *For any invertible matrix A, cond$(A) \geq 1$.*

Proof.

$$\text{cond}(A) = \|A\| \left\|A^{-1}\right\| \geq \left\|AA^{-1}\right\| = \|I_n\| = 1.$$

□

Corollary 5. *For $A \in M_n$,*

$$\textit{cond}(A) = 1$$

if and only if A is a scalar multiple of a unitary matrix.

Proof. ($\Rightarrow$) Assume

$$1 = \text{cond}(A) = \frac{\sigma_1}{\sigma_n}.$$

Then $\sigma_1 = \sigma_n$ and all singular values are equal. There are unitaries U and W such that

$$A = U \begin{pmatrix} \sigma_1 & & \\ & \ddots & \\ & & \sigma_1 \end{pmatrix} W^*$$

$$= \sigma_1 U I_n W^* = \sigma_1 U W^*$$

which is a scalar multiple of a unitary.

($\Leftarrow$) Suppose

$$A = \sigma U$$

where $\sigma \in \mathbb{C}$ and U is unitary. Then $\sigma = |\sigma| e^{i\theta}$ and

$$A = I_n \begin{pmatrix} |\sigma| & & \\ & \ddots & \\ & & |\sigma| \end{pmatrix} W^*,$$

where $W = e^{-i\theta} U^*$. Hence, the singular values of A are all equal to $|\sigma|$, and therefore $\text{cond}(A) = 1$.

□

Let $A \in M_n$ be given. From Theorem 7, it follows that σ_1, the largest singular value of A, is greater than or equal to the maximum Euclidean norm of the columns of A, and σ_n, the smallest singular value of A, is less than or equal to the minimum Euclidean norm of the columns of A by Corollary 6 and Corollary 2. If A is nonsingular we have shown that

$$\text{cond}(A) = \frac{\sigma_1}{\sigma_n},$$

which is thus bounded from below by the ratio of the largest to the smallest Euclidean norms of the set of columns of A. Thus if a system of linear equations

$$Ax = b$$

is poorly scaled (that is the ratio of the largest to the smallest row and column norms is large), then the system must be ill conditioned. The following example indicates that this sufficient condition for ill conditioning is not necessary, however. An example of an ill conditioned matrix for which all the rows and columns have nearly the same norm is the following.

Example 2.

$$A = \begin{bmatrix} 1 & -1 \\ -1 & 1+x \end{bmatrix}$$

$$B = \begin{bmatrix} 1 & -1 \\ 1 & -1+x \end{bmatrix}$$

$$A^{-1} = \begin{bmatrix} \frac{1+x}{x} & \frac{1}{x} \\ \frac{1}{x} & \frac{1}{x} \end{bmatrix}$$

$$B^{-1} = \begin{bmatrix} \frac{-1+x}{x} & \frac{1}{x} \\ \frac{-1}{x} & \frac{1}{x} \end{bmatrix}$$

The inverses indicate that as x approaches 0 the matrix conditions for A and B are of order $\frac{1}{x}$.

$$\text{cond}(A) = O(x^{-1})$$

$$\text{cond}(B) = O(x^{-1})$$

This is because the inverses diverge as x approaches zero.

$$\lim_{x \to 0}(A^{-1}) = O(x^{-1})$$

and

$$\lim_{x \to 0}(B^{-1}) = O(x^{-1})$$

since $\text{cond}(A) \equiv \begin{cases} \left\|A^{-1}\right\| \|A\|, & \text{if } A \text{ is nonsingular;} \\ \infty, & \text{if } A \text{ is singular} \end{cases}$.

This example shows that A and B are ill conditioned since a small perturbation (x) causes drastic change in the inverses of the matrices. This is in spite of all the rows and columns having nearly the same norm.

Least squares optimization application of the SVD will be discussed later and a computation example carried out using MATLAB to demonstrate the effect of the matrix condition on least squares approximation.

3.5 A norm approach to the singular values decomposition

In this section we establish a singular value decomposition using a matrix norm argument.

Theorem 9. *Let $A \in M_{m,n}$ be given, and let $q = min(m,n)$. There is a matrix $\Sigma = [\sigma_{i,j}] \in M_{m,n}$ with $\sigma_{i,j} = 0$ for all $i \neq j$, and $\sigma_{11} \geq \sigma_{22} \cdots \geq \sigma_{qq} \geq 0$, and there are two unitary matrices $V \in M_m$ and $W \in M_n$ such that $A = V\Sigma W^*$. If $A \in M_{m,n}(\mathbb{R})$, then V and W may be taken to be real orthogonal matrices.*

Proof. The Euclidean unit sphere in $\mathbb{C}^n$ is a compact set (closed and bounded) and the function $f(x) = \|Ax\|_2$ is a continuous real-valued function. Since a continuous real-valued function attains its maximum on a compact set, there is some unit vector $w \in \mathbb{C}^n$ such that

$$\|Aw\|_2 = \max\{\|Ax\|_2 : x \in \mathbb{C}^n,\ \|x\|_2 = 1\}.$$

If $\|Aw\| = 0$, then $A = 0$ and the factorization is trivial with $\Sigma = 0$ and any unitary matrices $V \in M_m$, $W \in M_n$. If $\|Aw\|_2 \neq 0$, set $\sigma_1 \equiv \|Aw\|_2$ and form the unit vector

$$v = \frac{Aw}{\sigma_1} \in \mathbb{C}^m.$$

There are $m-1$ orthonormal vectors $v_2, \cdots, v_m \in \mathbb{C}^m$ so that $V_1 \equiv [v\, v_2 \cdots v_m] \in M_m$ is unitary and there are $n-1$ orthonormal vectors vectors $w_2, \cdots, w_n \in \mathbb{C}^n$ so that

$W_1 \equiv [w\, w_2 \, \cdots \, w_n] \in M_n$ is unitary. Then

$$\begin{aligned}
\tilde{A}_1 \equiv V_1^* A W_1 &= \begin{bmatrix} v^* \\ v_2^* \\ \vdots \\ v_m^* \end{bmatrix} \begin{bmatrix} Aw & Aw_2 & \cdots & Aw_n \end{bmatrix} \\
&= \begin{bmatrix} v^* \\ v_2^* \\ \vdots \\ v_m^* \end{bmatrix} \begin{bmatrix} \sigma_1 v & Aw_2 & \cdots & Aw_n \end{bmatrix} \\
&= \begin{bmatrix} \sigma_1 & v^* A w_2 & \cdots & v^* A w_n \\ 0 & & & \\ \vdots & & A_2 & \\ 0 & & & \end{bmatrix} \\
&= \begin{bmatrix} \sigma_1 & z^* \\ 0 & A_2 \end{bmatrix},
\end{aligned}$$

where

$$z = \begin{bmatrix} w_2^* A^* v \\ \vdots \\ w_n^* A^* v \end{bmatrix} \in \mathbb{C}^{n-1},$$

and $A_2 \in M_{m-1,n-1}$.

Now consider the unit vector

$$\xi \equiv \frac{1}{(\sigma_1^2 + z^* z)^{\frac{1}{2}}} \begin{bmatrix} \sigma_1 \\ z \end{bmatrix} \in \mathbb{C}^n.$$

Then

$$\begin{aligned}
\tilde{A}_1 \xi &= \frac{1}{(\sigma_1^2 + z^* z)^{\frac{1}{2}}} \begin{bmatrix} \sigma_1 & z^* \\ 0 & A_2 \end{bmatrix} \begin{bmatrix} \sigma_1 \\ z \end{bmatrix} \\
&= \frac{1}{(\sigma_1^2 + z^* z)^{\frac{1}{2}}} \begin{bmatrix} \sigma_1^2 + z^* z \\ A_2 z \end{bmatrix},
\end{aligned}$$

so that

$$\left\|\tilde{A}_1\xi\right\|^2 = \frac{(\sigma_1^2 + z^*z)^2 + \|A_2z\|^2}{\sigma_1^2 + z^*z}.$$

Since V_1 is unitary, it then follows that

$$\|A(W_1\xi)\|^2 = \|V_1^*AW_1\xi\|^2 = \left\|\tilde{A}_1\xi\right\|^2 = \frac{(\sigma_1^2 + z^*z)^2 + \|A_2z\|^2}{\sigma_1 + z^*z} \geq \sigma_1^2 + z^*z.$$

This is greater than σ_1^2 if $z \neq 0$. This contradicts the construction assumption of

$$\sigma_1 = \max\{\|Ax\|_2 : x \in \mathbb{C}^n,\ \|x\|_2 = 1\}$$

and we conclude that $z = 0$. Then

$$\tilde{A}_1 = V_1^*AW_1 = \begin{bmatrix} \sigma_1 & 0 \\ 0 & A_2 \end{bmatrix}.$$

This argument is repeated on $A_2 \in M_{m-1,n-1}$ and the unitary matrices V and W are the *direct sums* ($\oplus$) of each step's unitary matrices:

$$A = V_1(I_1 \oplus V_2)\begin{bmatrix} \sigma_1 & & \\ & \sigma_2 & \\ & & A_3 \end{bmatrix}(I_1 \oplus W_2^*)W_1^*$$

$$= V_1(I_1 \oplus V_2)(I_2 \oplus V_3)\begin{bmatrix} \sigma_1 & & & \\ & \sigma_2 & & \\ & & \sigma_3 & \\ & & & A_4 \end{bmatrix}(I_2 \oplus W_3^*)(I_1 \oplus W_2^*)W_1^*,$$

etc. Since the matrix is finite dimensional, this process necessarily terminates, giving the desired decomposition. The result of this construction is $\Sigma = [\sigma_{ij}] \in M_{m,n}$ with $\sigma_{ii} = \sigma_i$ for $i = 1, \cdots, q$.

If $m \leq n$,

$$AA^* = V\Sigma\Sigma^TV^*$$

and

$$\Sigma\Sigma^T = \mathrm{diag}(\sigma_1^2, \cdots, \sigma_q^2).$$

If $m \geq n$, then A^*A leads to the same results. $\square$

When A is square and has distinct singular values the construction in the proof of Theorem 9 shows that

$$\sigma_1(A) = \max\{\|Ax\|_2 : x \in \mathbb{C}^n, \|x\|_2 = 1\} = \|Aw_1\|_2$$

for some unit vector $w_1 \in \mathbb{C}^n$,

$$\sigma_2(A) = \max\{\|Ax\|_2 : x \in \mathbb{C}^n, \|x\|_2 = 1,\ x \perp w_1\} = \|Aw_2\|$$

for some unit vector $w_2 \in \mathbb{C}^n$ with $w_2 \perp w_1$. In general,

$$\sigma_k(A) = \max\{\|Ax\|_2 : x \in \mathbb{C}^n, \|x\|_2 = 1, x \perp w_1, \cdots, w_{k-1}\},$$

so that $\sigma_k = \|Aw_k\|$ for some unit vector $w_k \in \mathbb{C}^n$ such that $w_k \perp w_1, \cdots, w_{k-1}$. This indicates that the maximum of $\|Ax\|_2$, with $\|x\| = 1$, and the the spectral norm of A coincide and are both equal to σ_1. Each singular value is the norm of A as a mapping restricted to a suitable subspace of $\mathbb{C}^n$.

3.6 Some matrix SVD inequalities

In this section we next examine some singular value inequalities.

Theorem 10. *Let $A = [a_{ij}] \in M_{m,n}$ have a singular value decomposition*

$$A = V\Sigma W^*$$

with unitaries $V = [v_{ij}] \in M_m$ and $W = [w_{ij}] \in M_n$, and let $q = \min(m, n)$. Then

(a.)

$$a_{ij} = v_{i1}\bar{w}_{j1}\sigma_1(A) + \cdots + v_{ik}\bar{w}_{jk}\sigma_k(A);$$

(b.)

$$\sum_{i=1}^{q} |a_{ii}| \leq \sum_{k=1}^{q}\sum_{i=1}^{q} |v_{ik}w_{ik}|\,\sigma_k(A) \leq \sum_{k=1}^{q} \sigma_k(A);$$

(c.)

$$Re\, tr\, A \leq \sum_{i=1}^{n} \sigma_i(A) \ for\ m = n,$$

with equality if and only if A is positive semidefinite;

Proof. (a.) Below we will use the notation $\mathbf{0}$ to indicate a block of zeros within a matrix. We first assume $m > n$ so $q = n$.

$$A = V\Sigma W^*$$

is of the form

$$A = [v_{ij}]\,\Sigma\,[w_{ij}]^*$$

with

$$\Sigma = \begin{bmatrix} \sigma_1(A) & & & \\ & \sigma_2(A) & & \\ & & \ddots & \\ & & & \sigma_q(A) \\ \mathbf{0} & \mathbf{0} & \cdots & \mathbf{0} \end{bmatrix}.$$

$$A = \begin{bmatrix} v_{11} & v_{12} & \cdots & v_{1m} \\ \vdots & \vdots & & \vdots \\ v_{m1} & v_{m2} & \cdots & v_{mm} \end{bmatrix} \begin{bmatrix} \sigma_1(A) & & & \\ & \sigma_2(A) & & \\ & & \ddots & \\ & & & \sigma_q(A) \\ \mathbf{0} & \mathbf{0} & \cdots & \mathbf{0} \end{bmatrix} \begin{bmatrix} \bar{w_{11}} & \bar{w_{21}} & \cdots & \bar{w_{n1}} \\ \vdots & \vdots & & \vdots \\ \bar{w_{1n}} & \bar{w_{2n}} & \cdots & \bar{w_{nn}} \end{bmatrix}$$

The first matrix (V) is an $m \times m$ matrix , the second (Σ) is an $m \times n$ matrix, and the third (W^*) is an $n \times n$ matrix. Multiplying Σ and W^* gives

$$A = \begin{bmatrix} v_{11} & v_{12} & \cdots & v_{1m} \\ \vdots & \vdots & & \vdots \\ v_{m1} & v_{m2} & \cdots & v_{mm} \end{bmatrix} \begin{bmatrix} \sigma_1(A)\bar{w_{11}} & \cdots & \sigma_1(A)\bar{w_{n1}} \\ \sigma_2(A)\bar{w_{12}} & \cdots & \sigma_2(A)\bar{w_{n2}} \\ \vdots & & \vdots \\ \sigma_q(A)\bar{w_{1q}} & \cdots & \sigma_q(A)\bar{w_{nq}} \\ \mathbf{0} & \cdots & \mathbf{0} \end{bmatrix}.$$

The first matrix above is V and the second one is an $m \times n$ matrix. If $n > m$ the last matrix above is of the form

$$\begin{bmatrix} \sigma_1(A)\bar{w_{11}} & \cdots & \sigma_1(A)\bar{w_{n1}} & \mathbf{0} \\ \sigma_2(A)\bar{w_{12}} & \cdots & \sigma_2(A)\bar{w_{n2}} & \mathbf{0} \\ \vdots & & \vdots & \mathbf{0} \\ \sigma_q(A)\bar{w_{1q}} & \cdots & \sigma_q(A)\bar{w_{nq}} & \mathbf{0} \end{bmatrix}.$$

The matrix product above leads to:

$$a_{11} = v_{11}\sigma_1(A)\bar{w}_{11} + v_{12}\sigma_2(A)\bar{w}_{12} + \cdots v_{1k}\sigma_q(A)\bar{w}_{1q}$$

and

$$a_{12} = v_{11}\sigma_1(A)\bar{w}_{21} + \cdots + v_{1q}\sigma_q(A)\bar{w}_{2q}.$$

In general,

$$a_{ij} = v_{i1}\sigma_1(A)\bar{w}_{j1} + \cdots + v_{iq}\sigma_q(A)\bar{w}_{jq},$$

where q is the rank of the matrix A. This gives (a.).

For (b.), set $i = j$ in

$$a_{ij} = v_{i1}\sigma_1(A)\bar{w}_{j1} + \cdots + v_{iq}\sigma_q(A)\bar{w}_{jq}$$

to get

$$a_{ii} = v_{i1}\sigma_1(A)\bar{w}_{i1} + \cdots + v_{iq}\sigma_q(A)\bar{w}_{iq}$$

or

$$a_{ii} = \sum_{k=1}^{q} v_{ik}\bar{w}_{ik}\sigma_k(A).$$

Taking magnitudes, the magnitude of a sum is less than or equal to the sum of the magnitudes (triangle inequality):

$$|a_{ii}| \leq \sum_{k=1}^{q} |v_{ik}\bar{w}_{ik}|\, \sigma_k(A).$$

summing both sides

$$\sum_{i=1}^{q} |a_{ii}| \leq \sum_{k=1}^{q} \sum_{i=1}^{q} |v_{ik} \bar{w}_{ik}| \, \sigma_k(A).$$

From the polar form of a complex number,

$$|v_{ik} \bar{w_{ik}}| = |v_{ik} w_{ik}|$$

since $\left|e^{i\theta}\right| = \left|e^{-i\theta}\right| = 1$. This leads to

$$\sum_{i=1}^{q} |a_{ii}| \leq \sum_{k=1}^{q} \sum_{i=1}^{q} |v_{ik} w_{ik}| \, \sigma_k(A) = \sum_{k=1}^{q} \sum_{i=1}^{q} |v_{ik}| \, |w_{ik}| \, \sigma_k(A).$$

For any k,

$$\sum_{i=1}^{q} |v_{ik}| \, |w_{ik}| \, \sigma_k(A) = \sigma_k(A) \sum_{i=1}^{q} |v_{ik}| \, |w_{ik}| = \sigma_k(A) \left[|v_{1k}| \cdots |v_{qk}| \right] \begin{bmatrix} |w_{1k}| \\ \vdots \\ |w_{qk}| \end{bmatrix}$$

$$= \sigma_k(A) \left\langle \begin{bmatrix} |v_{1k}| \\ \vdots \\ |v_{qk}| \end{bmatrix}, \begin{bmatrix} |w_{1k}| \\ \vdots \\ |w_{qk}| \end{bmatrix} \right\rangle.$$

By the Cauchy-Schwartz inequality, this is less than or equal to

$$\sigma_k(A) \left\| \begin{bmatrix} |v_{ik}| \\ \vdots \\ |v_{qk}| \end{bmatrix} \right\| \left\| \begin{bmatrix} |w_{1k}| \\ \vdots \\ |w_{qk}| \end{bmatrix} \right\| \leq \sigma_k(A) \cdot 1 \cdot 1 = \sigma_k(A).$$

Therefore,

$$\sum_{i=1}^{q} |a_{ii}| \leq \sum_{k=1}^{q} \sum_{i=1}^{q} |v_{ik} w_{ik}| \, \sigma_k(A) = \sum_{k=1}^{q} \sum_{i=1}^{q} |v_{ik}| \, |w_{ik}| \, \sigma_k(A) \leq \sum_{k=1}^{q} \sigma_k(A),$$

which proves (b.).

For (c.),

$$\operatorname{tr} A = \sum_{i=1}^{n} a_{ii}.$$

Then,

$$\operatorname{Re}\operatorname{tr} A = \sum_{i=1}^{n} \operatorname{Re}(a_{ii}) \leq \sum_{i=1}^{n} |a_{ii}| \leq \sum_{i=1}^{n} \sigma_i(A)$$

from (b.). This leads to

$$\operatorname{Re}\operatorname{tr} A \leq \sum_{i=1}^{n} \sigma_i(A).$$

For the second statement in part (c.), by part (a.)

$$\operatorname{tr} A = \sum_{i=1}^{n} a_{ii} = \sum_{i=1}^{n}\sum_{k=1}^{n} v_{ik}\bar{w}_{ik}\sigma_k(A) = \sum_{k=1}^{n}\left(\sum_{i=1}^{n} v_{ik}\bar{w}_{ik}\right)\sigma_k(A) = \sum_{k=1}^{n} \langle v_k, w_k\rangle\, \sigma_k(A),$$

where v_k and w_k are the k^{th} columns of V and W, respectively. Now, if

$$\operatorname{Re}\ \operatorname{tr}\ A = \sum_{i=1}^{n} \sigma_i(A),$$

then

$$\begin{aligned}
\sum_{k=1}^{n} \sigma_k(A) &= \sum_{k=1}^{n} \operatorname{Re}\ \langle v_k, w_k\rangle\, \sigma_k(A) = \left|\sum_{k=1}^{n} \operatorname{Re}\ \langle v_k, w_k\rangle\, \sigma_k(A)\right| \\
&\leq \sum |\operatorname{Re}\ \langle v_k, w_k\rangle|\, \sigma_k(A) \leq \sum |\langle v_k, w_k\rangle|\, \sigma_k(A) \\
&\leq \sum_{k=1}^{n} \|v_k\|\, \|w_k\|\, \sigma_k(A) \leq \sum_{k=1}^{n} \sigma_k(A)
\end{aligned}$$

by the triangle inequality and Cauchy-Schwarz inequality, respectively. Since the far left and the far right sides of this string of inequalities are equal, it follows that all the expressions are equal. Hence,

$$\sum_{k=1}^{n} \operatorname{Re}\ \langle v_k, w_k\rangle\, \sigma_k(A) = \sum |\operatorname{Re}\ \langle v_k, w_k\rangle|\, \sigma_k(A) = \sum_{k=1}^{n} \sigma_k(A).$$

Since $|\operatorname{Re}\langle v_k, w_k\rangle| \leq 1$ and $\sigma_k(A) \geq 0$, it follows that $\operatorname{Re}\ \langle v_k, w_k\rangle = 1$. It also follows that $\langle v_k, w_k\rangle = 1 = \|v_k\|\, \|w_k\|$. Equality in the Cauchy-Schwarz inequality implies that v_k is a scalar multiple of w_k, where the constant is of modulus one. Since also $\langle v_k, w_k\rangle = 1$, we must have $v_k = w_k$. Therefore $V = W$ and $A = V\Sigma W^* = V\Sigma V^*$, which is positive semidefinite since it is Hermitian and all eigenvalues are positive.

Conversely, if A is positive semidefinite, then the singular values are the same as the eigenvalues. Hence,

$$\operatorname{Re}\operatorname{tr} A = \operatorname{tr} A = \sum_{i=1}^{n} \sigma_i(A).$$

$\square$

3.7 Matrix polar decomposition and matrix SVD

We next examine the polar decomposition of a matrix using the singular value decomposition, and deduce the singular value decomposition from the polar decomposition of a matrix.

A singular value decomposition of a matrix can be used to factor a square matrix in a way analogous to the factoring of a complex number as the product of a complex number of unit length and a nonnegative number. The unit-length complex number is replaced by a unitary matrix and the nonnegative number by positive semidefinite matrix.

Theorem 11. *For any square matrix A there exists a unitary matrix W and a positive semidefinite matrix P such that*

$$A = WP.$$

Furthermore, if A is invertible, then the representation is unique.

Proof. By the singular decomposition, there exists unitary matrices U and V and a diagonal matrix Σ with nonnegative diagonal entries such that

$$A = U\Sigma V^*.$$

Thus

$$A = U\Sigma V^* = UV^*V\Sigma V^* = WP,$$

where $W = UV^*$ and $P = V\Sigma V^*$. Since W is the product of unitary matrices, W is unitary, and since Σ is positive semidefinite and P is unitarily equivalent to Σ, P is positive semidefinite.

Now suppose that A is invertible and factors as the products

$$A = WP = ZQ,$$

where W and Z are unitary, and P and Q are positive semidefinite (actually definite, since A is invertible). Since A is invertible it follows that P and Q are invertible and therefore,

$$Z^*W = QP^{-1}.$$

Thus QP^{-1} is unitary , and so

$$I = (QP^{-1})^*(QP^{-1}) = P^{-1}Q^2P^{-1}.$$

Hence by multiplying by P twice, this leads to $P^2 = Q^2$. Since both are positive definite it then follows that $P = Q$ by Lemma 1. Thus $W = Z$ and the factorization is unique.

The above factorization of a square matrix A as WP where W is unitary and P is positive definite is called a *polar decomposition of A.*

□

We use another theorem below to extend the polar decomposition to a matrix $A \in M_{m,n}$.

Theorem 12. *Let $A \in M_{m,n}$ be given.*

(a) If $n \geq m$, then $A = PY$, where $P \in M_m$ is positive semidefinite , $P^2 = AA^*$, and $Y \in M_{m,n}$ has orthonormal rows.

(b) If $m \geq n$, then $A = XQ$, where $Q \in M_n$ is positive semidefinite , $Q^2 = A^*A$, and $X \in M_{m,n}$ has orthonormal columns.

(c) If $m = n$, then $A = PU = UQ$, where $U \in M_n$ is unitary, $P, Q \in M_n$ are positive semidefinite, $P^2 = AA^*$, and $Q^2 = A^*A$.

The positive semidefinite factors P and Q are uniquely determined by A and their eigenvalues are the same as the singular values of A.

Proof. (a) If $n \geq m$ and

$$A = V\Sigma W^*$$

is a singular value decomposition , write

$$\Sigma = [S \quad 0],$$

with S the first m columns of Σ, and write

$$W = [W_1 \quad W_2],$$

where W_1 is the first m columns of W. Hence, $S = \mathrm{diag}(\sigma_1(A) \cdots \sigma_m(A)) \in M_m$ and $W_1 \in M_{n,m}$ and has orthonormal columns. Then

$$A = V[S \quad 0][W_1 \quad W_2]^* = VSW_1^* = (VSV^*)(VW_1^*).$$

Define $P = VSV^*$, so that $A = PVW_1^*$ and P is positive semidefinite. Also let $Y = VW_1^*$. Then

$$YY^* = VW_1^*W_1V^* = VI_mV^* = I_m$$

and so Y has orthonormal rows. Multiplying A by A^* yields

$$AA^* = (VSV^*)(VW_1^*)(VW_1^*)^*(VSV^*)^* = (VSV^*)^2 = P^2,$$

since

$$(VW_1^*)(VW_1^*)^* = I.$$

For (b), the case $m \geq n$, we apply part (a) to A^*, so that $A^* = PY$ where $P^2 = A^*(A^*)^* = A^*A$, P is positive semidefinite, and Y has orthonormal rows. Then $A = Y^*P$. Let $X = Y^*$ and $Q = P$. Then $A = XQ$, X has orthonormal columns, $Q^2 = A^*A$ and is positive semidefinite.

For (c),

$$A = V\Sigma W^* = (V\Sigma V^*)(VW^*) = (VW^*)(W\Sigma W^*).$$

Take $P = V\Sigma V^*$, $Q = W\Sigma W^*$, and $U = VW^*$ with

$$A = PU = UQ.$$

Moreover, U is unitary, P and Q are positive semidefinite, and $P^2 = AA^*$ and $Q^2 = A^*A$. □

We next consider a theorem and corollaries that examine some of the special matrix classes by using singular value decomposition.

3.8 The SVD and special classes of matrices

Definition 15. *A matrix $C \in M_n$ is a* ***contraction*** *if $\sigma_1(C) \leq 1$ (and hence $0 \leq \sigma_i(C) \leq 1$ for all $i = 1, 2, \cdots, n$).*

Definition 16. *A matrix $P \in M_{m,n}$ is said to be a rank r* ***partial isometry*** *if $\sigma_1(P) = \cdots = \sigma_r(P) = 1$ and $\sigma_{r+1}(P) = \cdots = \sigma_q(P) = 0$, where $q \equiv min(m,n)$. Two partial isometries $P, Q \in M_{m,n}$ (of unspecified rank) are said to be* ***orthogonal*** *if $P^*Q = 0$ and $PQ^* = 0$.*

Theorem 13. *Let $A \in M_{m,n}$ have singular value decomposition $A = V\Sigma W^*$ with $V = [v_1 \cdots v_m] \in M_m$ and $W = [w_1 \cdots w_n] \in M_n$ unitary, and $\Sigma = [\sigma_{ij}] \in M_{m,n}$ with $\sigma_1 = \sigma_{11} \geq \cdots \geq \sigma_q = \sigma_{qq} \geq 0$ and $q = \min(m,n)$.*
Then

(a.) $A = \sigma_1 P_1 + \cdots + \sigma_q P_q$ *is a nonnegative linear combination of mutually orthogonal rank one partial isometries, with $P_i = v_i w_i^*$ for $i = 1, \cdots, q$.*

(b.) $A = \mu_1 K_1 + \cdots + \mu_q K_q$ *is a nonnegative linear combination of mutually orthogonal partial isometries K_i with rank $i = 1, \cdots, q$, such that*

  (i.) $\mu_i = \sigma_i - \sigma_{i+1}$ *for $i = 1, \cdots, q-1$,* $\mu_q = \sigma_q$.

  (ii.) $\mu_i + \cdots + \mu_q = \sigma_i$ *for $i = 1, \cdots, q$, and*

  (iii.) $K_i = VE_iW^*$ *for $i = 1, \cdots, q$ in which the first i columns of $E_i \in M_{m,n}$ are the respective unit basis vectors $e_1, \cdots, e_i$ and the remaining $n - i$ columns are zero.*

Proof. (a) From Theorem 10, we have shown that for a matrix $A \in M_{m,n}$

$[a_{ij}] = [v_{i1}\bar{w}_{j1}\sigma_1(A) + \cdots + v_{ik}\bar{w}_{jk}\sigma_k(A)]$, where $A = V\Sigma W^*$ with unitary $V = [v_{ij}] \in M_m$ and $W = [w_{ij}] \in M_n$, and with $q = \min(m,n)$. Let

$$v_1 = \begin{bmatrix} v_{11} \\ \vdots \\ v_{m1} \end{bmatrix}$$

and

$$w_1 = \begin{bmatrix} w_{11} \\ \vdots \\ w_{n1} \end{bmatrix}.$$

Then

$$w_1^* = \begin{bmatrix} \bar{w}_{11} & \cdots & \bar{w}_{n1} \end{bmatrix}.$$

Let

$$P_1 = v_1 w_1^* = \begin{bmatrix} v_{11} \\ \vdots \\ v_{m1} \end{bmatrix} \begin{bmatrix} \bar{w}_{11} & \cdots & \bar{w}_{n1} \end{bmatrix} = \begin{bmatrix} v_{11}\bar{w}_{11} & \cdots & v_{11}\bar{w}_{n1} \\ \vdots & & \vdots \\ v_{m1}\bar{w}_{11} & \cdots & v_{m1}\bar{w}_{n1} \end{bmatrix}.$$

More generally, let

$$P_i = v_i w_i^* = \begin{bmatrix} v_{1i} \\ \vdots \\ v_{mi} \end{bmatrix} \begin{bmatrix} \bar{w}_{1i} & \cdots & \bar{w}_{ni} \end{bmatrix} = \begin{bmatrix} v_{1i}\bar{w}_{1i} & \cdots & v_{1i}\bar{w}_{ni} \\ \vdots & & \vdots \\ v_{mi}\bar{w}_{1i} & \cdots & v_{mi}\bar{w}_{ni} \end{bmatrix}$$

for $i = 1, \cdots, q$. The above P_i matrices are all $m \times n$ matrices and the (i,j)-entry of

$$\sigma_1 P_1 + \cdots + \sigma_q P_q,$$

is given by

$$v_{i1}\bar{w}_{j1}\sigma_1(A) + \cdots + v_{ik}\bar{w}_{jk}\sigma_k(A),$$

where k is the rank of the matrix A. Since $k \leq q$, if $q > k$ there will be $q-k$ zero singular values and summation to k will give the same results as summation to q. Therefore

$$A = [a_{ij}] = [v_{i1}\bar{w}_{j1}\sigma_1(A) + \cdots + v_{iq}\bar{w}_{jq}\sigma_q(A)],$$

and

$$A = \sigma_1 P_1 + \cdots + \sigma_q P_q.$$

To show that P_i is a rank one partial isometry,

$$P_1 = v_1 w_1^* = V \begin{bmatrix} 1 & 0 & \ldots & 0 \\ 0 & 0 & \ldots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & \cdots & 0 & 0 \end{bmatrix}.$$

In general,

$$P_i = V F_i W^*,$$

where F_i is the matrix with a 1 in the i^{th} diagonal entry and zeros everywhere else. Thus, P_i is a rank 1 partial isometry. For $i \neq j$,

$$P_i^* P_j = (V F_i W^*)(V F_j W^*) = W F_i F_j W^* = 0.$$

Thus the P_i's are mutually orthogonal. For (b.), let $\mu_i = \sigma_i - \sigma_{i+1}$ for $i = 1, \cdots, q-1$, and $\mu_q = \sigma_q$. This leads to a telescoping sum:

$$\mu_i + \cdots + \mu_q = \sigma_q + \sum_{j=i}^{q-1} (\sigma_j - \sigma_{j+1}) = \sigma_1 \quad \text{for } i = 1, \cdots, q,$$

because of mutual cancelation of the middle terms. Now define

$$K_i = V E_i W^*.$$

Then each K_i is a rank i partial isometry. By part (a.) (and it's proof),

$$\begin{aligned} A &= \sigma_1 P_1 + \cdots + \sigma_q P_q \\ &= (\mu_1 + \cdots + \mu_q) P_1 + (\mu_2 + \cdots + \mu_q) P_2 + \cdots + \mu_q P_q \\ &= \mu_1 P_1 + \mu_2 (P_1 + P_2) + \mu_3 (P_1 + P_2 + P_3) + \cdots + \mu_q (P_1 + \cdots + P_q) \\ &= \mu_1 K_1 + \cdots + \mu_q K_q, \end{aligned}$$

since $K_i = P_1 + \cdots + P_i$.

$\square$

Corollary 6. *The unitary matrices are the only rank n (partial) isometries in M_n.*

Proof. Let $A \in M_n$ be unitary. Then

$$A^*A = I_n,$$

and the eigenvalues of $I_n = A^*A$ are n ones. Then taking the square root leads to n singular values $\sigma_i(A)$= 1 for all $i = 1, \ldots, n$. Thus, A is a rank n partial isometry.

On the other hand, let $B \in M_n$ be any rank n partial isometry. Then

$$B = VI_nW^*$$

is the singular value decomposition of B. It follows that

$$B = VW^*,$$

which is unitary (a product of unitaries). Thus B is unitary. Since any unitary matrix $A \in M_n$ is unitary and any rank n partial isometry matrix $B \in M_n$ is unitary, then it follows that the unitary matrices are the only rank n (partial) isometries in M_n.

$\square$

Theorem 14. *If $C \in M_n$ is a contraction and $y \in \mathbb{C}^n$ with $\|y\| \leq 1$, then $\|Cy\| \leq 1$. Conversely, if $\|Cy\| \leq 1$, for any $y \in \mathbb{C}^n$ with $\|y\| \leq 1$, then C is a contraction.*

Proof. Let

$$C = V\Sigma W^*$$

be a singular value decomposition. Since W^* is unitary,

$$\|W^*y\| = \|y\| \leq 1.$$

Let z_i be the i^{th} component of W^*y. Then

$$\Sigma W^*y = \begin{bmatrix} \sigma_1 z_1 \\ \vdots \\ \sigma_n z_n \end{bmatrix}.$$

Hence,

$$\|\Sigma W^* y\| = \sqrt{|\sigma_1 z_1|^2 + \cdots + |\sigma_n z_n|^2} \leq \sqrt{|z_1|^2 + \cdots + |z_n|^2} \leq 1.$$

Since V is unitary,

$$\|V\Sigma W^* y\| = \|\Sigma W^* y\| \leq 1.$$

Thus,

$$\|Cy\| \leq 1.$$

For the converse, let $y \in \mathbb{C}^n$ such that $W^* y = e_1$. Then $\|y\| = 1$ and

$$\sigma_1 = \left\| \begin{bmatrix} \sigma_1 \\ 0 \\ \vdots \\ 0 \end{bmatrix} \right\| = \|\Sigma e_1\| = \|\Sigma W^* y\| = \|V\Sigma W^* y\| = \|Cy\| \leq 1.$$

Thus C is a contraction. $\square$

Corollary 7. *Any finite product of contractions is a contraction.*

Proof. Let $\|y\| \leq 1$, and let C_1 and C_2 be any contractions, then

$$\|C_1 C_2 y\| \leq \|C_2 y\| \leq \|y\| \leq 1.$$

By the converse of the theorem above,

$$\sigma_1(C_1 C_2) \leq 1.$$

By induction, the result holds for any finite product of contractions. $\square$

Corollary 8. *$C \in M_n$ is a rank one partial isometry if and only if $C = vw^*$ for some unit vectors $v, w \in \mathbb{C}^n$.*

Proof. $(\Rightarrow)$ Assume $C \in M_n$ is a rank one partial isometry. Then

$$
\begin{aligned}
C &= V\Sigma W^* = V \begin{bmatrix} 1 & & & \\ & 0 & & \\ & & \ddots & \\ & & & 0 \end{bmatrix} W^* \\
&= \begin{bmatrix} v_{11} & v_{12} & \cdots & v_{1n} \\ v_{21} & v_{22} & \cdots & v_{2n} \\ \vdots & \vdots & & \vdots \\ v_{n1} & v_{n2} & \cdots & v_{nn} \end{bmatrix} \begin{bmatrix} 1 & \cdots & 0 \\ \vdots & & \vdots \\ 0 & \cdots & 0 \end{bmatrix} \begin{bmatrix} \bar{w}_{11} & \bar{w}_{21} & \cdots & \bar{w}_{n1} \\ \bar{w}_{12} & \bar{w}_{22} & \cdots & \bar{w}_{n2} \\ \vdots & \vdots & & \vdots \\ \bar{w}_{1n} & \bar{w}_{2n} & \cdots & \bar{w}_{nn} \end{bmatrix} \\
&= \begin{bmatrix} v_{11} & 0 & \cdots & 0 \\ v_{21} & 0 & \cdots & 0 \\ \vdots & & & \vdots \\ v_{n1} & & \cdots & 0 \end{bmatrix} \begin{bmatrix} \bar{w}_{11} & \cdots & \bar{w}_{n1} \\ \vdots & & \vdots \\ \bar{w}_{1n} & \cdots & \bar{w}_{nn} \end{bmatrix} \\
&= \begin{bmatrix} v_{11}\bar{w}_{11} & v_{11}\bar{w}_{21} & \cdots & v_{11}\bar{w}_{n1} \\ \vdots & \vdots & & \vdots \\ v_{n1}\bar{w}_{11} & v_{n2}\bar{w}_{21} & \cdots & v_{n1}\bar{w}_{n1} \end{bmatrix} \\
&= \begin{bmatrix} v_{11} \\ v_{21} \\ \vdots \\ v_{n1} \end{bmatrix} \begin{bmatrix} \bar{w}_{11} & \bar{w}_{21} & \cdots & \bar{w}_{n1} \end{bmatrix} \\
&= vw^*.
\end{aligned}
$$

This proves that if $C \in M_n$ is a rank one partial isometry, then $C = vw^*$ for some unit vectors $v, w \in \mathbb{C}^n$.

($\Leftarrow$) Suppose $C = vw^*$, for unit vectors $v, w \in \mathbb{C}^n$. Extend $\{v\}$ and $\{w\}$ to orthonormal bases $\{v_1, v_2 \cdots, v_n\}$ and $\{w_1, w_2, \cdots, w_n\}$ of $\mathbb{C}^n$. Let $V = [v_1\ v_2 \cdots v_n]$ and

$W = [w_1 \ w_2 \cdots w_n]$. Then

$$C = VW^* = V \begin{bmatrix} 1 & & & & \\ & 0 & & & \\ & & 0 & & \\ & & & \ddots & \\ & & & & 0 \end{bmatrix} W,$$

so C is a rank one partial isometry. $\square$

Corollary 9. *For $1 \leq r < n$, every rank r partial isometry in M_n is a convex combination of two unitary matrices in M_n.*

Proof. Let A be a rank r partial isometry in M_n. There exist unitaries V, W such that

$$A = VE_rW^*,$$

with

$$E_r = \begin{bmatrix} I_r & 0 \\ 0 & 0 \end{bmatrix} \in M_n.$$

Then

$$E_r = \frac{1}{2}\left[(I_r \oplus I_{n-r}) + (I_r \oplus (-I_{n-r}))\right]$$

so that

$$\begin{aligned} A &= V\left\{\frac{1}{2}\left[(I_r \oplus I_{n-r}) + (I_r \oplus (-I_{n-r}))\right]\right\}W^* \\ &= \frac{1}{2}V(I_r \oplus I_{n-r})W^* + \frac{1}{2}V(I_r \oplus (-I_{n-r}))W^*. \end{aligned}$$

Since $V(I_r \oplus I_{n-r})W^*$ and $V(I_r \oplus (-I_{n-r}))W^*$ are unitary, the proof is complete. $\square$

Corollary 10. *Every matrix in M_n is a finite nonnegative linear combination of unitary matrices in M_n.*

Proof. From Theorem 13

$$A = \sigma_1 P_1 + \cdots + \sigma_n P_n,$$

where each P_i is a partial isometry. This leads to a nonnegative linear combination of unitary matrices in M_n, since each P_i is a convex combination of unitary matrices by Corollary 9, and the singular values σ_i are nonnegative. □

Corollary 11. *A contraction in M_n is a finite convex combination of unitary matrices in M_n.*

Proof. Assume that $A \in M_n$ is a contraction. By Theorem 13,

$$A = \mu_1 K_1 + \cdots + \mu_n K_n$$

where $\mu_1 + \cdots + \mu_n = \sigma_1$ and each K_i is a rank i partial isometry in M_n. By Corollary 9 and its proof, we can write

$$K_i = \left(\frac{1}{2}U_i + \frac{1}{2}V_i\right),$$

where U_i and V_i are unitaries. Since A is a contraction, then $\sigma_1(A) \leq 1$. Since $\mu_1 + \cdots + \mu_n = \sigma_1$, if $\sigma_1 = 1$, then A is a convex combination of unitary matrices in M_n:

$$A = \sum_{i=1}^{n} \mu_i \left[\frac{1}{2}U_i + \frac{1}{2}V_i\right] = \sum_{i=1}^{n} \frac{\mu_i}{2}U_i + \frac{\mu_i}{2}V_i.$$

If $\sigma_1 < 1$, then we can write

$$A = \sum_{i=1}^{n} \left[\frac{\mu_i}{2}U_i + \frac{\mu_i}{2}V_i\right] + (1 - \sigma_i)\left[\frac{1}{2}I_n + \frac{1}{2}(-I_n)\right].$$

The sum of the coefficients is

$$\sum_{i=1}^{n} \frac{\mu_i}{2} + \frac{\mu_i}{2} + (1 - \sigma_1) = \sigma_1 + (1 - \sigma_1) = 1.$$

Hence, A is a convex combination of unitaries. □

3.9 The pseudoinverse

Let V and W be finite-dimensional inner product spaces over the same field, and let $T : V \to W$ be a linear transformation. We recall that for a linear transformation to be invertible, it must be a one-to-one function and also onto. If the null space ($N(T)$) has one or more nonzero vectors $x \in N(T)$ such that

$$T(x) = 0,$$

then T is not invertible. Since being invertible is a desirable property, a simple approach to dealing with noninvertible transformations or matrices is to focus on the part of T that is invertible by restricting T to $N(T)^{\perp}$. Let $L : N(T)^{\perp} \to R(T)$ be a linear transformation defined by

$$L(x) = T(x) \quad \text{for} \quad x \in N(T)^{\perp}.$$

Then L is invertible since it is restricted to $N(T)^{\perp}$. We can use the inverse of L to construct a linear transformation from W to V, in the reverse direction, that has some of the benefits of an inverse of T.

Definition 17. *Let V and W be finite-dimensional inner product spaces over the same field, and let $T : V \to W$ be a linear transformation. Let $L : N(T)^{\perp} \to R(T)$ be the linear transformation defined by*

$$L(x) = T(x) \quad \forall x \in N(T)^{\perp}.$$

The pseudoinverse (or Moore-Penrose generalized inverse) of T, denoted $T^{\dagger}$, is defined as the unique linear transformation from W to V such that

$$T^{\dagger}(y) = \begin{cases} L^{-1}(y), & \textit{for } y \in R(T) \\ 0, & y \in R(T)^{\perp}. \end{cases}$$

The pseudoinverse of a linear transformation T on a finite-dimensional inner product space exists even if T is not invertible. If T is invertible, then $T^{\dagger} = T^{-1}$ because $N(T)^{\perp} = V$ and L, as defined above, coincides with T.

Theorem 15. *Let $T : V \to W$ be a linear transformation and let $\sigma_1 \geq \cdots \geq \sigma_n$ be the nonzero singular values of T. Then there exist orthonormal bases $\{v_1, \ldots, v_n\}$ and $\{u_1, \ldots, u_m\}$ for V and W, respectively, and a number r, $0 \leq r \leq m$, such that*

$$T^{\dagger}(u_i) = \begin{cases} \frac{1}{\sigma_i} v_i, & \text{if } 1 \leq i \leq r \\ 0, & \text{if } r < i \leq m. \end{cases}$$

Proof. By Theorem 3 (Singular Value Theorem), there exist orthonormal bases $\{v_1, \ldots, v_n\}$ and $\{u_1, \ldots, u_m\}$ for V and W, respectively, and nonzero scalars $\sigma_1 \geq \cdots \geq \sigma_r$ (the nonzero singular values of T), such that

$$T(v_i) = \begin{cases} \sigma_i u_i, \text{ if } 1 \leq i \leq r, \text{ and} \\ 0, \text{ if } \; i > r. \end{cases}$$

Since the σ_i are nonzero, it follows that $\{v_1, \cdots, v_r\}$ is an orthonormal basis for $N(T)^{\perp}$ and that $\{v_{r+1}, \cdots, v_n\}$ is an orthonormal basis for $N(T)$. Since T has rank r, it also follows that $\{u_1, \cdots, u_r\}$ and $\{u_{r+1}, \cdots, u_m\}$ are orthonormal bases for $R(T)$ and $R(T)^{\perp}$, respectively. Here $R(T)$ denotes the range of T.

Let L be the restriction of T to $N(T)^{\perp}$. Then

$$L^{-1}(u_i) = \frac{1}{\sigma_i} v_i \quad \text{for } 1 \leq i \leq r.$$

Therefore

$$T^{\dagger}(u_i) = \begin{cases} \frac{1}{\sigma_i} v_i, & \text{if } 1 \leq i \leq m \\ 0, & \text{if } r < i \leq m. \end{cases}$$

□

We will see quite a bit more of the pseudoinverse in Section 5.

3.10 Partitioned matrices and the outer product form of the SVD

This subsection is an application of Theorem 13 and Corollary 8. The outer rows and columns of the matrix Σ can be eliminated if the matrix product $A = U\Sigma V^T$ is expressed using partitioned matrices as follows:

$$A = \left[\begin{array}{ccc|ccc} u_1 & \cdots & u_k & u_{k+1} & \cdots & u_m \end{array}\right] \left[\begin{array}{ccc|c} \sigma_1 & & & \\ & \ddots & & 0 \\ & & \sigma_k & \\ \hline & 0 & & 0 \end{array}\right] \left[\begin{array}{c} {v_1}^T \\ \vdots \\ {v_k}^T \\ \hline {v_{k+1}}^T \\ \vdots \\ {v_n}^T \end{array}\right]$$

When the partitioned matrices are multiplied, the result is

$$A = \left[\begin{array}{ccc} u_1 & \ldots & u_k \end{array}\right] \left[\begin{array}{ccc} \sigma_1 & & \\ & \ddots & \\ & & \sigma_k \end{array}\right] \left[\begin{array}{c} v_1^T \\ \vdots \\ {v_k}^T \end{array}\right] \oplus \left[\begin{array}{ccc} u_{k+1} & \ldots & u_m \end{array}\right] \left[\begin{array}{c} 0 \end{array}\right] \left[\begin{array}{c} {v_{k+1}}^T \\ \vdots \\ {v_n}^T \end{array}\right]$$

It is clear that only the first k of the u_i and v_i make any contribution to A. We can shorten the equation to

$$A = \left[\begin{array}{ccc} u_1 & \ldots & u_k \end{array}\right] \left[\begin{array}{ccc} \sigma_1 & & \\ & \ddots & \\ & & \sigma_k \end{array}\right] \left[\begin{array}{c} v_1^T \\ \vdots \\ {v_k}^T \end{array}\right]$$

The matrices of u_i and v_i are now rectangular $(m \times k)$ and $(k \times n)$ respectively. The diagonal matrix is square. This is an alternative formulation of the SVD. Thus we have established the following proposition.

Proposition 8. *Any $m \times n$ matrix A of rank k can be expressed in the form $A = U\Sigma V^T$ where U is an $m \times k$ matrix such that $U^T U = I_k$, Σ is a $k \times k$ diagonal matrix with positive entries in decreasing order on the diagonal, and V is an $n \times k$ matrix such that $V^T V = I_k$.*

Usually in a matrix product XY, the rows of X are multiplied by the columns of Y. In the outer product expansion, a column is multiplied by a row, so with X an $m \times k$

matrix and Y a $k \times n$ matrix

$$XY = \sum_{i=1}^{k} x_i {y_i}^T,$$

where the x_i are the columns of X and y_i^T are the rows of Y. Let

$$X = \begin{bmatrix} u_1 & \dots & u_k \end{bmatrix} \begin{bmatrix} \sigma_1 & & \\ & \ddots & \\ & & \sigma_k \end{bmatrix} = \begin{bmatrix} \sigma_1 u_1 & \dots & \sigma_k u_k \end{bmatrix}$$

and

$$Y = \begin{bmatrix} {v_1}^T \\ \vdots \\ {v_k}^T \end{bmatrix}.$$

Then $A = XY$ can be expressed as an outer product expansion

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

Thus, for a vector x,

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

since ${v_i}^T x$ is a scalar, this leads to (change of order)

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

Ax is expressed as a linear combination of the vectors u_i. Each coefficient is a product of the two factors, ${v_i}^T x$ and σ_i, with ${v_i}^T x = \langle x, v_i \rangle$, which is the i^{th} component of x relative to the orthonormal basis $\{v_1, \dots, v_n\}$. Under the action of A each v component of x becomes a u component after scaling by the appropriate σ.

4 The SVD and systems of linear equations

4.1 Linear least squares

For the remaining sections we will work exclusively with the real scalar field. Suppose we have a linearly independent set of vectors and wish to combine them linearly to provide the best possible approximation to a given vector. If the set is $\{a_1, a_2, \ldots, a_n\}$ and the given vector is b, we seek coefficients $x_1, x_2, \ldots, x_n$ that produce a minimal error

$$\left\| b - \sum_{i=1}^{n} x_i a_i \right\| .$$

Using finite columns of numbers, define an $m \times n$ matrix A with columns given by a_i, and a vector x whose entries are the unknown coefficients x_i. We want to choose x minimizing

$$\| b - Ax \| .$$

Equivalently, we seek an element of the subspace S spanned by the a_i that is closest to b. This is given by the orthogonal projection of b onto S. This projection of b onto S is characterized by the fact that the vector difference between b and its projection should be orthogonal to S. Thus the solution vector x must satisfy

$$\langle a_i, (Ax - b) \rangle = 0, \quad \text{for } i = 1, \cdots, n.$$

In matrix form this becomes

$$A^T(Ax - b) = 0.$$

This leads to

$$A^T A x = A^T b.$$

This set of equations for the x_i are referred to as the *normal equations* for the linear least squares problem. Since $A^T A$ is invertible (due to linear independence of the columns of A) this leads to

$$x = (A^T A)^{-1} A^T b.$$

Numerically, the formation of $(A^T A)^{-1}$ can degrade the accuracy of a computation, since the formation of the inverse numerically is often only an approximation.

Turning to an SVD solution for the least squares problem, we can avoid the need for calculating the inverse of $A^T A$.

We again wish to choose x so that we minimize

$$\|Ax - b\|.$$

Let

$$A = U\Sigma V^T$$

be a SVD for A, where U and V are are square orthogonal matrices, and Σ is rectangular with the same dimensions as A $(m \times n)$. Then

$$\begin{aligned} Ax - b &= U\Sigma V^T x - b \\ &= U(\Sigma V^T x) - U(U^T b) \\ &= U(\Sigma y - c), \end{aligned}$$

where $y = V^T x$ and $c = U^T b$.

Since U is orthogonal (preserves length),

$$\|U(\Sigma y - c)\| = \|\Sigma y - c\|.$$

Hence,

$$\|Ax - b\| = \|\Sigma y - c\|.$$

We now seek y to minimize the norm of the vector $\Sigma y - c$.

Let the components of y be y_i for $1 \leq i \leq n$. Then

$$\Sigma y = \begin{bmatrix} \sigma_1 y_1 \\ \vdots \\ \sigma_k y_k \\ 0 \\ 0 \\ \vdots \\ 0 \end{bmatrix},$$

so that

$$\Sigma y - c = \begin{bmatrix} \sigma_1 y_1 - c_1 \\ \vdots \\ \sigma_k y_k - c_k \\ -c_{k+1} \\ -c_{k+2} \\ \vdots \\ -c_m \end{bmatrix}.$$

It is easily seen that, when

$$y_i = \frac{c_i}{\sigma_i}$$

for $1 \le i \le k$, $\Sigma y - c$ assumes its minimal length which is given by

$$\left[\sum_{i=k+1}^{n} c_i^2 \right]^{\frac{1}{2}}.$$

To solve the least squares problem:

1. Determine the SVD of A and calculate c as

$$c = U^T b$$

2. Solve the least squares problem for Σ and c that is find y so that

$$\|\Sigma y - c\|$$

is minimal. The diagonal nature of Σ makes this easy.

3. Since

$$y = V^T x,$$

which is equivalent to to

$$x = V y,$$

by left multiplying the above equation with V, this gives the solution x. The error is

$$\|\Sigma y - c\|.$$

The SVD has reduced the least squares problem to a diagonal form. In this form the solution is easily obtained.

Theorem 16. *The solution to the least squares problem described above is*

$$x = V\Sigma^{\dagger}U^T b,$$

where

$$A = U\Sigma V^T$$

is a singular value decomposition.

Proof. The solution from the normal equations is

$$x = \left(A^T A\right)^{-1} A^T b.$$

Since

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

then

$$x = (V\Sigma^T \Sigma V^T)^{-1}(U\Sigma V^T)^T b.$$

The inverse

$$(V\Sigma^T \Sigma V^T)^{-1}$$

is equal to

$$V(\Sigma^T \Sigma)^{-1} V^T.$$

The product

$$\Sigma^T \Sigma$$

is a square matrix whose k diagonal entries are the σ_i^2. Hence,

$$\begin{aligned} x &= V(\Sigma^T\Sigma)^{-1}V^T(U\Sigma V^T)^T b \\ &= V(\Sigma^T\Sigma)^{-1}V^T V\Sigma^T U^T b. \end{aligned}$$

Since $V^T V = I_n$,

$$\begin{aligned} x &= V(\Sigma^T\Sigma)^{-1}\Sigma^T U^T b \\ &= V\Sigma^\dagger U^T b. \end{aligned}$$

The last equality follows because$(\Sigma^T\Sigma)^{-1}$ is equal to a square matrix whose diagonal elements are equal to $\frac{1}{\sigma_i^2}$ combined with $\Sigma^T = \Sigma$ which has σ_i as the diagonal elements. The matrix $\Sigma^\dagger$ has diagonal elements of $\frac{1}{\sigma_i}$ and is the pseudoinverse of the matrix Σ. $\square$

4.2 The pseudoinverse and systems of linear equations

Let $A \in M_{m,n}(\mathbb{R})$ be a matrix. For any $b \in \mathbb{R}^m$

$$Ax = b$$

is a system of linear equations. The system of linear equations either has no solution, has a unique solution, or has infinitely many solutions. A unique solution exists for every $b \in \mathbb{R}^m$ if and only if A is invertible. In this case, the solution is

$$x = A^{-1}b = A^\dagger b.$$

If we do not assume that A is invertible, but suppose that $Ax = b$ has a unique solution for a particular b, then that solution is given by $A^\dagger b$ (Theorem 17).

Lemma 2. *Let V and W be finite-dimensional inner product spaces, and let $T : V \to W$ be linear. Then*

(a.) $T^\dagger T$ is the orthogonal projection of V onto $N(T)^\perp$

(b.) $TT^\dagger$ is the orthogonal projection of W onto $R(T)$.

Proof. Define $L : N(T)^\perp \to W$ by

$$L(x) = T(x) \quad \text{for} \quad x \in N(T)^\perp.$$

Then for $x \in N(T)^\perp$, $T^\dagger T(x) = L^{-1}L(x) = x$. If $x \in N(T)$, then $T^\dagger T(x) = T^\dagger(0) = 0$. Thus $T^\dagger T$ is the orthogonal projection of V onto $N(T)^\perp$, which gives (a.).

If $x \in N(T)^\perp$ and $y = T(x) \in R(T)$, then $TT^\dagger(y) = T(x) = y$. If $y \in R(T)^\perp$, then $T^\dagger(y) = 0$, so that then $TT^\dagger(y) = 0$. This gives (b.). □

Theorem 17. *Consider the system of linear equations $Ax = b$, where A is an $m \times n$ matrix and $b \in \mathbb{R}^m$. If $z = A^\dagger b$, then z has the following properties.*

(a.) If $Ax = b$ is consistent, then z is the unique solution to the system having minimum norm. That is, z is a solution to the system and if y is any solution to the system, then $\|z\| \leq \|y\|$ with equality if and only if $z = y$.

(b.) If $Ax = b$ is inconsistent, then z is the unique best approximation to a solution having minimum norm. That is, $\|Az - b\| \leq \|Ay - b\|$ for any $y \in \mathbb{R}^n$, with equality if and only if $Az = Ay$. Furthermore, if $Az = Ay$, then $\|z\| \leq \|y\|$ with equality if and only if $z = y$.

Proof. For (a.), suppose $Ax = b$ is consistent, and $z = A^\dagger b$. Since $b \in R(A)$, the range of A, then $Az = AA^\dagger b = b.$, by the lemma above. Thus z is a solution of the system. If y is any solution to the system, then

$$A^\dagger A(y) = A^\dagger b = z.$$

Since z is the orthogonal projection of y onto $N(A)^\perp$, then $\|z\| \leq \|y\|$ with equality if and only if $z = y$.

For (b.), suppose $Ax = b$ is inconsistent, then by the above lemma $Az = AA^\dagger b$, which is the orthogonal projection of b onto $R(A)$. Thus Az is the vector in $R(A)$ nearest to b. Similarly, as in (a.), if Ay is any vector in $R(A)$, then $\|Az - b\| \leq \|Ay - b\|$ with equality if and only if $Az = Ay$. If $Az = Ay$, then $\|z\| \leq \|y\|$, with equality if and only if $z = y$. □

4.3 Computational considerations

Note the vector $z = A^\dagger b$ in the above theorem is the vector $x = V\Sigma^\dagger U^T b$, where $x = A^\dagger b$ using the SVD of A in the SVD application to the least squares problem above. From this discussion the result using the normal equations

$$x = (A^T A)^{-1} A^T b$$

and the result using the SVD

$$x = V \Sigma^{\dagger} U^T b$$

should give the same result for the solution of the least squares problem. It turns out that in computations with matrices, the effects of limited precision (due to machine representation of numbers with a limited precision or number of digits) depend on the *condition number* of a matrix. A large condition number for a matrix is a sign that a numerical instability will occur in solutions of linear systems.

In the computation using the SVD

$$\Sigma^{\dagger}$$

is multiplied by $U^T b$. In comparison; using the normal equations

$$(A^T A)^{-1}$$

is multiplied by $A^T b$.

The eigenvalues of $A^T A$ (λ_i) are the squares of the singular values of A (σ_i)

Thus

$$\frac{\lambda_1}{\lambda_n} = \left(\frac{\sigma_1}{\sigma_n} \right)^2 .$$

The condition number of $A^T A$ is the square of the condition number of A.

Thus when computing with $A^T A$ you need roughly twice as many digits to be as accurate as when you compute with the SVD of A (see Kalman(1996) [6]).

At this point we need to emphasize that there are algorithms for determining the SVD of a matrix without using eigenvalues and eigenvectors; one such algorithm is the Rayleigh-Ritz principle. See [4]. This is essential to avoid the pitfall of the instability that may occur from the larger condition number of $A^T A$ in comparison to that of A for some matrices as described above. There are algorithms for computing the SVD using implicit matrix computation methods. The basic idea of one of such algorithms for computing the SVD of A is to use the EVD of $A^T A$. A sequence of approximations for $A_i = U_i \Sigma_i V_i^T$ to the desired correct SVD of A are made. The validity of the SVD algorithm is then established by ensuring that after each iteration , the product $A_i^T A_i$ is what is produced by a well known algorithm for the EVD of $A^T A$. The convergence of the SVD is determined by the EVD, without computing $A^T A$ in full. The SVD algorithm is then an implicit method for the EVD of $A^T A$. The operations on A are seen to implicitly form the EVD algorithm for $A^T A$, without ever explicitly forming $A^T A$. See [6]. We illustrate this condition number discussion. Starting with an example with a very high matrix condition number ([6]), we then modify the data to obtain a lower condition number. A comparison of the errors is made by calculating the magnitude of the residual

$$\|b - Ax\|$$

using the SVD and then using the normal equations (via $A^T A$). We do the calculations in MATLAB. First define (in MATLAB notation)

$$c1 = [1\,2\,4\,8]'$$

and

$$c2 = [3\,6\,9\,12]'.$$

Then define a third vector as:

$$c3 = c1 - 4 * c2 + 0.0000001 * rand((4,1) - 0.5 * [1\,1\,1\,1]')$$

and the matrix A is defined to have these three vectors as its columns

$$A = [c1 \quad c2 \quad c3]$$

The command rand(4,1) returns a four entry column vector with entries randomly chosen between 0 and 1. Subtracting 0.5 from each entry shifts them between $\frac{-1}{2}$ and $\frac{1}{2}$. The b vector is defined in a similar way by adding a small random vector to a specified linear combination of columns of A.

$$b = 2 * c1 - \ 7 * c2 \ + \ 0.0001 * (rand(4,1) \ - 0.5 * [1\,1\,1\,1]')$$

The SVD of A is determined by the MATLAB command

$$[U, \quad S, \quad V] = svd(A)$$

Here, the three matrices U, S ($S \equiv \Sigma$), and V are displayed on the screen and also kept in the computer memory.

$$59.810,\ 2.5976\,\text{and}\,1.0578 \times 10^{-8}$$

are the singular values (σ_i) resulting from running the commands. This indicates a condition number

$$\left(\frac{\sigma_1}{\sigma_n}\right) = \frac{59.810}{1.0578 \times 10^{-8}} = 6 \times 10^9.$$

To compute $\Sigma^\dagger$, we need to transpose the diagonal matrix S and invert the non-zero diagonal entries. This matrix is denoted by G. The matrix G consists of the diagonal reciprocal of the diagonal elements of matrix S. The matrix S represents the matrix of singular values Σ as defined above. Thus G represents the pseudoinverse of Σ denoted by $\Sigma^\dagger$ above.

$$\begin{aligned} G &= S' \qquad (3) \\ G(1,1) &= \frac{1}{S(1,1)} \\ G(2,2) &= \frac{1}{S(2,2)} \\ G(3,3) &= \frac{1}{S(3,3)} \end{aligned}$$

The SVD solution is given as:

$$x = V\Sigma^\dagger U^T b$$

Multiply this by A to get Ax and see how far this is from b; using the commands:

$$r1 = b - A * V * G * U' * b \tag{4}$$

$$e1 = sqrt(r1' * r1)$$

$$e1 = 2.5423 \times e^{-005} \tag{5}$$

This small magnitude indicates a satisfactory solution of the least squares problem using the SVD. The normal equations solution, in comparison, is as follows:

$$x = (A^T A)^{-1} A^T b$$

The MATLAB commands are:

$$r2 = b - \ A * inv(A' * A) * A' * b$$

$$e2 = sqrt(r2' * r2)$$

and MATLAB responds

$$e2 = 28.7904$$

The $e2$ is of the same order of magnitude as $|b| = 97.2317$. The solution using the normal equations does a poor job, in comparison to the SVD solution.

On the other hand, if we modify the starting vectors as follows

$$c4 = [24816]'$$

and

$$c5 = [481320]'$$

then using the same procedure in MATLAB we get the following siglular values

$$90.2178,\ 3.5695,\ \text{and}\, 0.0632.$$

This results in a condition number

$$\left(\frac{\sigma_1}{\sigma_n}\right) = \frac{90.2178}{0.0632} = 1.428 \times 10^3.$$

This condition number is 10^6 order of magnitude less than the one above (6×10^9).

The resulting errors calculated by SVD and by the normal equations are

$$e2 = 3.2414 \times e^{-006}$$

and the same value by the normal equations

$$e3 = 3.2514 \times e^{-006}.$$

This small magnitude indicates a satisfactory solution of the least squares problem using both the SVD and the normal equations in the case where the matrix condition number is not too high.

We next consider our last application, data compression.

5 Image compression using reduced rank approximations

5.1 The Frobenius norm and the outer product expansion

We recall the expression of the SVD in the outer product form, an application of Theorem 13 and section 3.10:

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

This is directly applicable to data compression. The above equation is applicable in a situation where an $m \times n$ matrix is approximated by using fewer numbers than the original $m \times n$ elements. Suppose a photograph is represented by an $m \times n$ matrix of pixels, each pixel assigned a gray level on a scale of 0 to 1. The rank of the matrix specifies the number of linearly independent columns (or rows). A matrix that has a low rank implies linear dependence of some of the rows (or columns). The linear dependence (redundancy) allows the matrix to be expressed more efficiently without storing all the matrix elements. Consider a rank one matrix. Instead of the $m \times n$ matrix, we can represent the matrix by $m + n$ numbers. A matrix B of rank one can be represented as:

$$B = [v_1 u \ v_2 u \cdots v_n u],$$

where $u \in \mathbb{R}^m$ and $v_1, \ldots, v_n \in \mathbb{R}$. Thus $B = uv^T$, where

$$v = \begin{bmatrix} v_1 \\ \vdots \\ v_n \end{bmatrix}.$$

This is a product of a column and a row, an *outer product*, as defined in section 3.10. The m entries of the column and the n entries of the row ($m + n$ numbers) represent the rank one matrix. If B is the best rank one approximation to A the error $B - A$ has a minimal Frobenius norm. The Frobenius norm of a matrix is defined as the square root of the sums of squares of its entries and is denoted by $\| \cdot \|_2$. The inner product of two matrices

$$X = [x_{ij}] \quad \text{and} \quad Y = [y_{ij}],$$

$$X \cdot Y = \sum_{ij} x_{ij} y_{ij}$$

can be thought of as the sum of the mn products of the corresponding entries.

Theorem 18. *The Frobenius norm of a real matrix is unaffected by multiplying either on the left or the right by an orthogonal matrix.*

Proof. Considering rank one matrices xy^T and uv^T:

$$\begin{aligned} xy^T \cdot uv^T &= [xy_1 \cdots xy_n] \cdot [uv_1 \cdots uv_n] \\ &= \sum_i xy_i \cdot uv_i \\ &= \sum_i (x \cdot u) y_i v_i \\ &= (x \cdot u)(y \cdot v). \end{aligned}$$

From the outer product expansion

$$XY = \sum_i X_i Y_i^T$$

(with X_i being the columns of X and Y_i^T the rows of Y), this leads to

$$\begin{aligned} (XY) \cdot (XY) &= (\sum_i x_i y_i^T) \cdot (\sum_j x_j y_j^T) \\ &= \sum_{ij} (x_i \cdot x_j)(y_i \cdot y_j), \end{aligned}$$

or

$$\|XY\|_2 = \sum_i \|x_i\|^2 \|y_i\|^2 + \sum_{i \neq j} (x_i \cdot x_j)(y_i \cdot y_j).$$

If the x_i are orthogonal, then

$$\|XY\|_2 = \sum \|x_i\|^2 \|y_i\|^2.$$

If the x_i are both orthogonal and of unit length, then

$$\|XY\|_2 = \sum_i \|y_i\|^2 = \|Y\|_2 .$$

A similar argument works when Y is orthogonal. The argument above indicates that Frobenius norm of a matrix is unaffected by multiplying on either the left or the right by an orthogonal matrix. $\square$

Corollary 12. *Given a matrix A with SVD $A = V\Sigma W^T$, then*

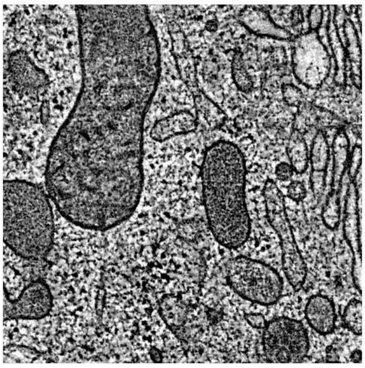
$$\|A\|_2^2 = \sum_i \sigma_i^2.$$

Proof. Let $A = V\Sigma W^T$ be a singular value decomposition. Then

$$\|A\|_2 = \|V\Sigma W^T\|_2 = \|\Sigma\|_2 = \sum_i \sqrt{\sigma_i^2},$$

since V and W are orthogonal matrices and make no difference to the Frobenius norm. $\square$

5.2 Reduced rank approximations to greyscale images

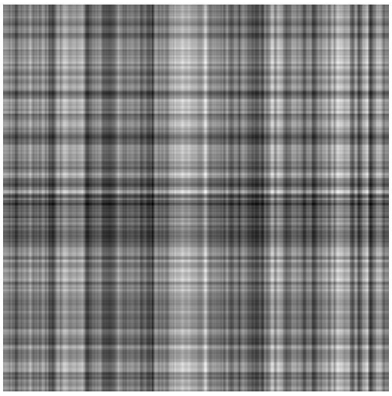


A greyscale image of a cell

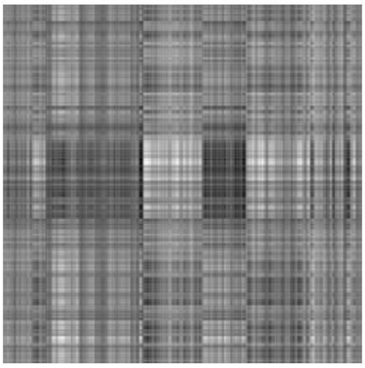
As discussed in the previous section, we may represent a greyscale image by a matrix. For example, the matrix representing the JPEG image above is a 512×512 matrix A which has rank $k = 512$. By using the outer product form

$$A = \sum_i^k \sigma_i u_i v_i^T,$$

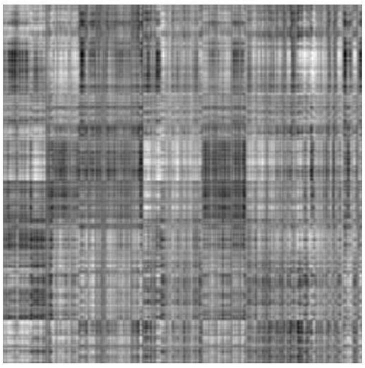
we obtain a reduced rank approximation by just summing the first $r \leq k$ terms. The images given below are a result of a MATLAB SVD program which makes reduced rank approximations of a greyscale picture. A graph of the magnitude of the singular values is also given. It indicates that the singular values decrease rapidly from the maximum singular value. By rank 12, the approximation of the picture begins to show enough structure to represent the original.



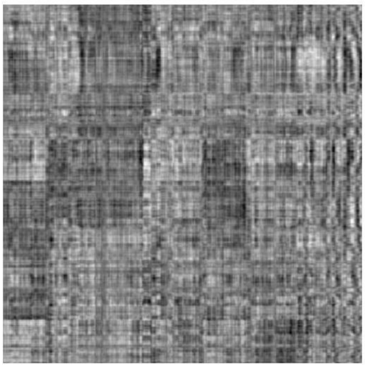
Rank 1 cell approximation



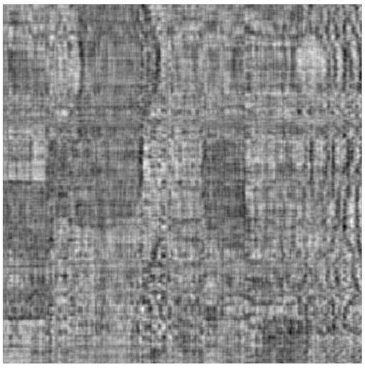
Rank 2 cell approximation



Rank 4 cell approximation

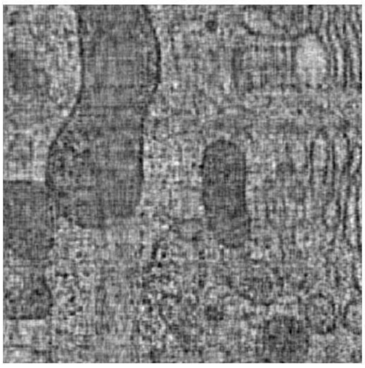


Rank 8 cell approximation

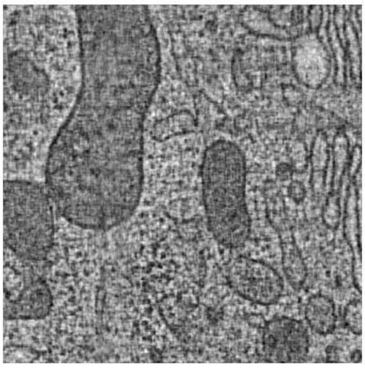


Rank 12 cell approximation

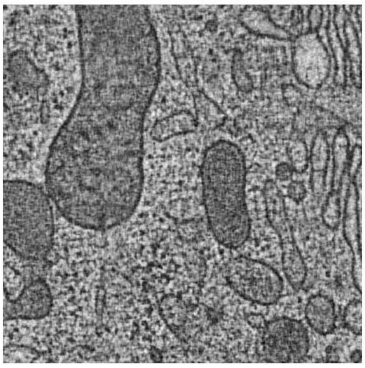
More detailed iterations resulting into higher rank for the cell picture are indicated below:



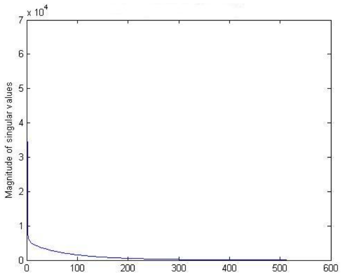
Rank 20 cell approximation



Rank 40 cell approximation



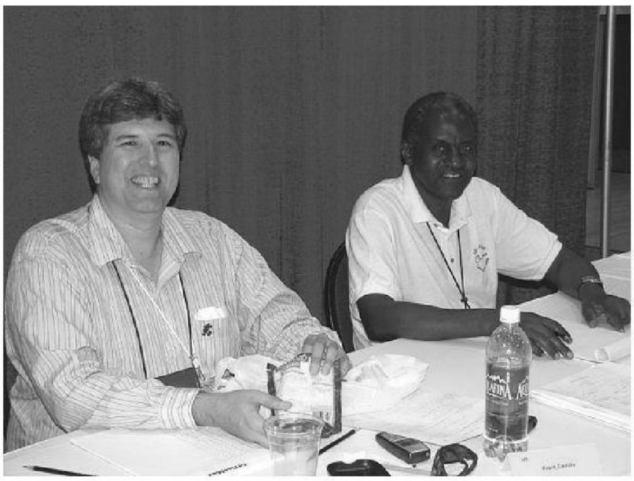
Rank 60 cell approximation



σ_i vs. i for the cell picture

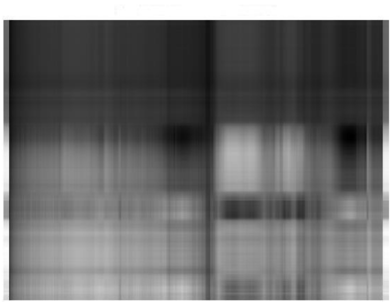
Two other images are processed by the MATLAB program indicated as Appendix 1. The first is a photograph of the thesis author in Fort Collins Colorado State University during AP Calculus reading (2007). The last image is a picture of waterlilies. It is necessary to have a MATLAB image processing tool box to run the MATLAB code provided in the appendix.

Calculus grading photograph



Grayscale image of the photograph

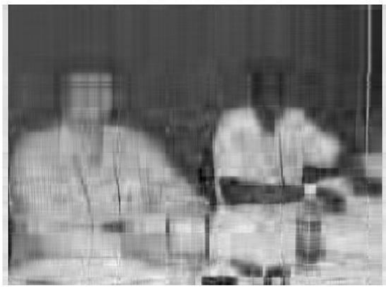
Rank 1 approximation of the image



Rank 2 approximation of the image

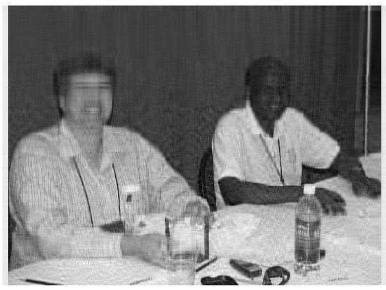
Rank 4 approximation of the image

Rank 8 approximation of the image



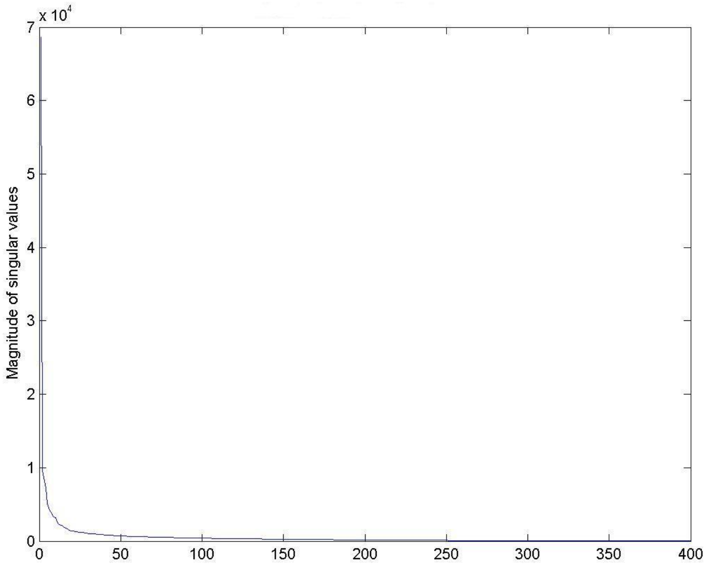
Rank 12 approximation of the image

Rank 20 approximation of the image

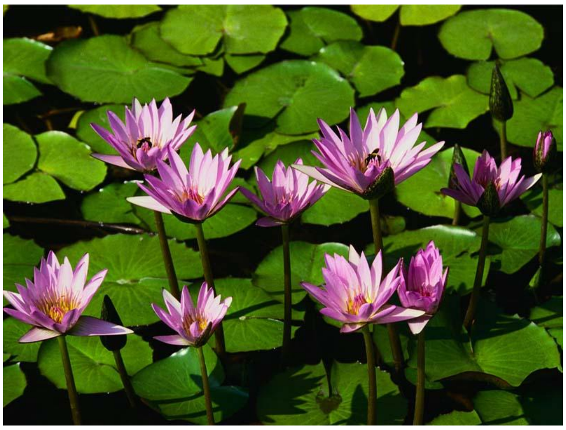


Rank 40 approximation of the image

Rank 60 approximation of the image

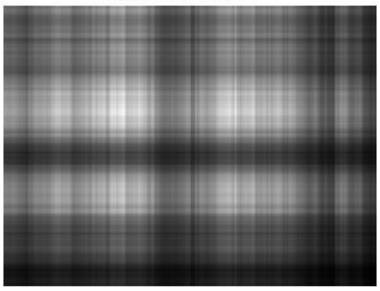


Singular value graph of the gray scale calculus grading photograph

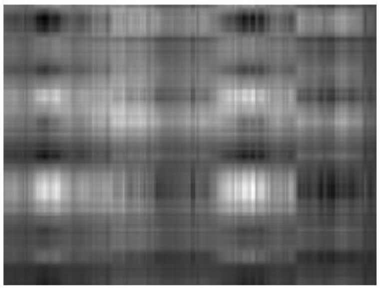


Sample photograph of waterlilies

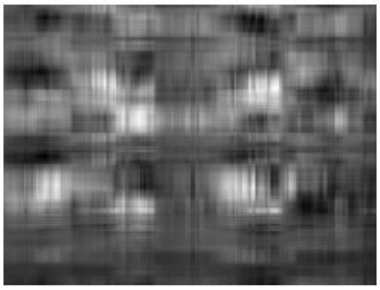
Gray scale image of waterlilies



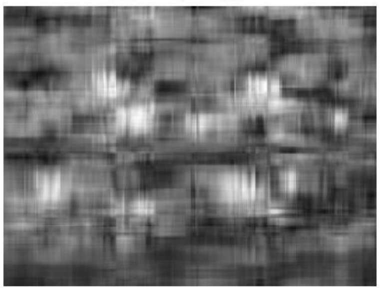
Rank 1 approximation of lilies image



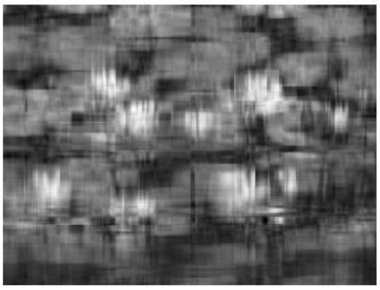
Rank 2 approximation of lilies image



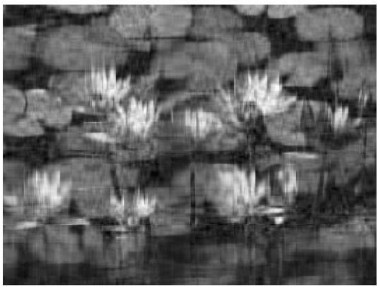
Rank 4 approximation of lilies image



Rank 8 approximation of lilies image



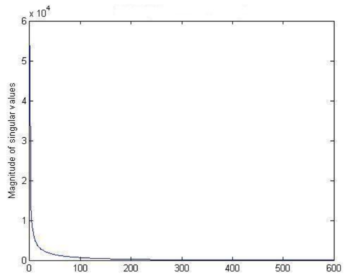
Rank 12 approximation of lilies image



Rank 20 approximation of lilies image

Rank 40 approximation of lilies image

Rank 60 approximation of lilies image



Singular values graph for the lilies image

5.3 Compression ratios

The images looked at so far have been stored as *JPEG* (*.jpg*) images which are already compressed. It is more appropriate to start with an uncompressed bitmap (*.bmp*) image to determine the efficiency of compression. The efficiency of compression can be quantified using the *compression ratio*, *compression factor*, or *saving percentage*. These are defined as follows:

1. *compression ratio*:

$$\frac{\text{size after compression}}{\text{size before compression}};$$

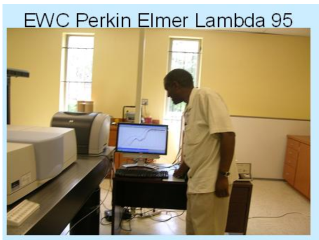
2. *compression factor*:

$$\frac{\text{size before compression}}{\text{size after compression}};$$

3. *saving percentage*:

$$\text{compression ratio} \times 100.$$

Consider the following image (bitmap) below. The image is 454 pixels long by 454 pixels wide, for a total of $206,116$ pixels.



Original image of the EWC Lab photograph

For a rank 16 approximation, the compression ratio is equal to

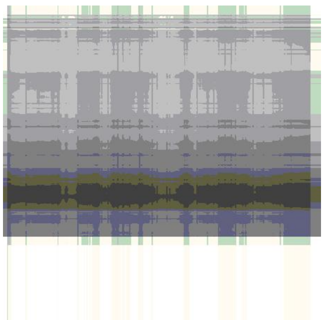
$$\frac{14544}{454 \times 454} = 0.07056,$$

which corresponds to a compression factor of 14.17189, and a saving percentage of about 7.1 %. The table below indicates the compression ratio and compression factor for eight ranks ranging from 1 to 128.

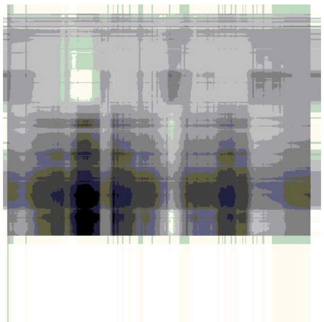
Rank	Compression Ratio	Saving Percentage
1	0.00441	0.441%
2	0.00882	0.82 %
4	0.0176	1.76 %
8	0.0353	3.53 %
16	0.0706	7.06 %
32	0.141	14.1 %
64	0.282	28.2 %
128	0.564	56.4 %

The corresponding images are given below.

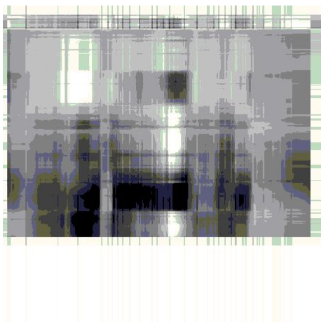
Grayscale image of the EWC Lab bit map photograph



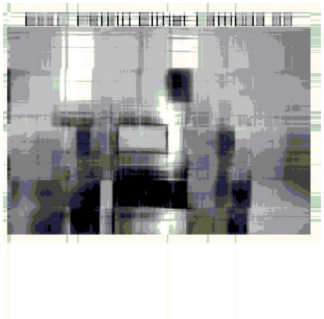
Rank 1



Rank 2



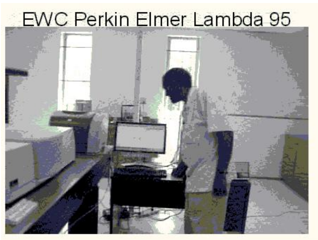
Rank 4



Rank 8

Rank 16

Rank 32



Rank 64

Rank 128

6 Conclusion

We have discussed some of the mathematical background to the singular value factorization of a matrix. There are many applications of the singular value decomposition. We have discussed three of those applications: least squares approximation, digital image compression using reduced rank matrix approximation, and the role of the pseudoinverse of a matrix in solving equations. The least squares approximation depends on the matrix condition number as demonstrated by computation using two different matrix condition numbers. The results of reduced rank image compression using MATLAB indicate that low rank image approximations produce reasonably identifiable images. The SVD low rank approximation provides a compressed image with reduced storage compression ratio of ten to fifty percent of the original file storage size. Our results for a *.bmp* image indicate that there is a large range of choice from an identifiable but poor image of rank 16 approximation to a high quality rank 128 image. The original input matrix for compression has full rank of 454. This corresponds to a choice of compression factors ranging from 7 % to 50%. Image fidelity sensitive applications like medical imaging can use the high end rank approximation. Other less fidelity sensitive applications, where it is just required to identify the image, can take advantage of the low end of the approximation. This is possible since the matrices Σ for all the images decay very fast as indicated by the graphs of the singular values σ_i as a function of i. Low rank approximations based on the largest first few singular values provide a sufficient approximation to the full matrix representation of the image.

A The MATLAB code used to perform rank approximation of the JPEG images

clear; close all;

fname=input(’Give file name within single quotes: ’); colorflag=input(’Enter 1 for a color image, 0 otherwise: ’);

I=imread(fname); if colorflag == 1 I=rgb2gray(I); end I=double(I);

figure(1) imshow(mat2gray(I)) title([’Gray scale version of ’ fname])

disp(’==’) disp(’We will now study the singular value decomposition of the image.’) disp(’ ’) disp(’Press any key to compute the singular value decomposition.’) pause disp(’Please wait...’)

[U S V]=svd(I,0);

disp(’The singular value decomposition has been computed.’) disp(’The output contains three matrices U, S and V.’) whos disp(’ ’) disp(’Press any key to continue’) pause

disp(’==’) disp(’We will now look at the singular values.’) disp(’The singular values are given along the diagonal of S.’) disp(’Notice the rapid decay!’)

figure(2) plot(diag(S)) title(’The singular values of the image’) ylabel(’Magnitude of singular values’)

disp(’ ’) disp(’Press any key to continue.’) pause

disp(’==’) disp(’The columns of U contain an orthogonal basis for the ’) disp(’column space of the image.’) disp(’The columns of V contain an orthogonal basis for the ’) disp(’row space of the image.’) disp(’ ’) disp(’Press any key to continue.’) pause

disp(’==’) disp(’Let us look at a rank one approximation of the image.’)

Ssp=sparse(S);

[M,N]=size(U); Utemp=zeros(M,N); Utemp(:,1)=U(:,1);

[M,N]=size(V); Vtemp=zeros(M,N); Vtemp(:,1)=V(:,1);

Irank1=Utemp*Ssp*Vtemp'; figure(3) imshow(mat2gray(Irank1)) title('A rank one approximation of the image')

disp('Note that all columns are just multiples of a single column vector!')

disp(' ') disp('Press any key to continue.') pause

disp('==') disp('Let us look at a rank two approximation of the image.')

[M,N]=size(U); Utemp=zeros(M,N); Utemp(:,1:2)=U(:,1:2);

[M,N]=size(V); Vtemp=zeros(M,N); Vtemp(:,1:2)=V(:,1:2);

Irank2=Utemp*Ssp*Vtemp'; figure(4) imshow(mat2gray(Irank2)) title('A rank two approximation of the image')

disp('All columns are linear combination of just two column vectors.')

disp(' ') disp('Press any key to continue.') pause

disp('==') disp('Let us look at a rank four approximation of the image.')

[M,N]=size(U); Utemp=zeros(M,N); Utemp(:,1:4)=U(:,1:4);

[M,N]=size(V); Vtemp=zeros(M,N); Vtemp(:,1:4)=V(:,1:4);

Irank4=Utemp*Ssp*Vtemp'; figure(5) imshow(mat2gray(Irank4)) title('A rank four approximation of the image')

disp('All columns are linear combination of just four column vectors.') disp('Despite using only four basis vectors, you should be able ') disp('to see some structure in your image.')

disp(' ') disp('Press any key to continue.') pause

disp('==') disp('Let us look at a rank eight approximation of the image.')

[M,N]=size(U); Utemp=zeros(M,N); Utemp(:,1:8)=U(:,1:8);

[M,N]=size(V); Vtemp=zeros(M,N); Vtemp(:,1:8)=V(:,1:8);

Irank8=Utemp*Ssp*Vtemp'; figure(6) imshow(mat2gray(Irank8)) title('A rank eight approximation of the image')

```
disp('All columns are linear combination of eight column vectors.')
disp(' ') disp('Press any key to continue.') pause
disp('=========================================')
disp('Now choose your own rank!') Nrank=input('Enter rank you want to study: ')
Ssp=sparse(S);
[M,N]=size(U); Utemp=zeros(M,N); Utemp(:,1:Nrank)=U(:,1:Nrank);
[M,N]=size(V); Vtemp=zeros(M,N); Vtemp(:,1:Nrank)=V(:,1:Nrank);
Irank=Utemp*Ssp*Vtemp'; figure(7) imshow(mat2gray(Irank))
title(['A rank ', num2str(Nrank), ' approximation of the image.'])
```

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