The Significance of Orthogonal Matrices[−1−].

A square matrix Q is *orthogonal* if

$$Q^T = Q^{-1}, \qquad \text{i.e.,} \qquad Q^T Q = QQ^T = I. \tag{1}$$

Hence $Q^{-1} = Q^T$, and an orthogonal matrix is invertible. Moreover, orthogonal matrices provide an exception (pretty much the only one) to our rule that you never invert a matrix.

Since the (i, j) entry of $Q^T Q$ is the dot product of the i-th and j-th columns of Q, it is clear that geometrically the columns (or rows) of an orthogonal matrix form an *orthonormal* set, i.e., a set of unit vectors that are pairwise orthogonal. Another way of looking at this is that the columns of an orthogonal matrix provide a basis of orthonormal vectors of $\mathbb{R}^n$, and that any such basis defines an orthogonal matrix.

Orthogonal matrices are used ubiquitously throughout Numerical Analysis because they **do not amplify errors**. To see this note that if Q is orthogonal then

$$\|Qx\|_2^2 = (Qx)^T Qx = x^T Q^T Qx = x^T x = \|x\|_2^2. \tag{2}$$

So if you build a numerical algorithm on multiplications with orthogonal matrices then errors present in the original problem will not be amplified by the algorithm.

The fact (2) has immediate consequences (think about it): The 2-norm[−2−] of an orthogonal matrix is 1, and any eigenvalue has absolute value equal to 1. The property (1) implies that the determinant of an orthogonal matrix is plus or minus 1:

$$\|Q\|_2 = 1, \qquad Qx = \lambda x \neq 0 \quad \Longrightarrow \quad |\lambda| = 1, \qquad \det Q = \pm 1. \tag{3}$$

It is also true that the product of orthogonal matrices is orthogonal.

Exercise 1. *Verify the claims made in this section. Find some orthogonal matrices.*

We will encounter many orthogonal matrices in the course of this semester, including the identity matrix, permutation matrices, reflection matrices, rotation matrices, and several factorizations involving orthogonal matrices. The first such factorization is

The Singular Value Decomposition.

What Is It.

Suppose we are given an $m \times n$ matrix A, where, usually,

$$m \geq n. \tag{4}$$

−1− by Peter Alfeld, 801-581-6842, JWB 127, pa@math.utah.edu. TEX processed on July 1, 2014.

−2− The norm of a matrix A is $\max_{x \neq 0} \|Ax\|/\|x\|$.

The *Singular Value Decomposition* of A is

$$\boxed{A = U\Sigma V^T} \tag{5}$$

where

- U is $m \times m$ orthogonal, i.e., $U^{-1} = U^T$,
- V is $n \times n$ orthogonal, i.e., $V^{-1} = V^T$, and
- Σ is $m \times n$ diagonal. Specifically,

$$\Sigma = \begin{bmatrix} \sigma_1 & 0 & \dots & 0 \\ 0 & \sigma_2 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & \sigma_n \\ 0 & 0 & \dots & 0 \\ \vdots & \vdots & & \vdots \\ 0 & 0 & \dots & 0 \end{bmatrix} \tag{6}$$

where

$$\sigma_1 \geq \sigma_2 \geq \ldots \geq \sigma_n \geq 0. \tag{7}$$

Note that Σ is a matrix! The capital Greek letter Σ in this context has nothing to do with the summation symbol[−3−]. The σ_i are the *singular values* of A. The columns of U and V are the *left* and *right*, respectively, *singular vectors* of A.

Some insight may be gained, and some of the mystery can perhaps be lifted, by observing that the right singular vectors of A are the eigenvectors of A^TA, and the singular values are the square roots of the corresponding eigenvalues of A^TA.

To see this let v_j be the j-th column of V and note that

$$A^T = V\Sigma^T U^T. \tag{8}$$

Letting

$$S = \Sigma^T\Sigma = \begin{bmatrix} \sigma_1^2 & 0 & \dots & 0 \\ 0 & \sigma_2^2 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & \sigma_n^2 \end{bmatrix} \tag{9}$$

−3− I first learned about the singular value decomposition in an excellent talk by Cleve Moler that I understood only in retrospect. At the time of that first exposure the talk was utterly wasted on me because the whole time I kept thinking *What is he summing there?* However, the notation $A = U\Sigma V^T$ is well established.

and e_j be the j-th unit vector. We obtain

$$\begin{aligned} A^T A v_j &= V\Sigma^T \underbrace{U^T U}_{=I} \Sigma \underbrace{V^T v_j}_{=e_j} \\ &= V\Sigma^T \Sigma e_j \\ &= V S e_j \\ &= \sigma_j^2 v_j \end{aligned} \tag{10}$$

which is what we want to show.

Existence.

Theorem. *Every matrix has a singular value decomposition.*

The following proof is taken (with little modification but a little elaboration) from Golub/van Loan, p. 76. Let $A \in \mathbb{R}^{m\times n}$, and let $x \in \mathbb{R}^n$ and $y \in \mathbb{R}^m$ be unit 2-norm vectors that satisfy

$$Ax = \sigma y \qquad \text{with} \qquad \sigma = \|A\|_2. \tag{11}$$

There exist matrices $V_2 \in \mathbb{R}^{n\times(n-1)}$ and $U_2 \in \mathbb{R}^{m\times(m-1)}$ such that

$$V = [x\ V_2] \quad \text{and} \quad U = [y\ U_2] \tag{12}$$

are orthogonal.
It is not hard to show that $U^T AV$ has the following structure:

$$U^T AV = \begin{bmatrix} \sigma & w^T \\ 0 & B \end{bmatrix} =: A_1. \tag{13}$$

Since

$$\|A_1\|_2^2 \left(\sigma^2 + w^T w\right) \geq \left\| A_1 \begin{bmatrix} \sigma \\ w \end{bmatrix} \right\|_2^2 \geq (\sigma^2 + w^T w)^2 \tag{14}$$

we have, after dividing by $\left(\sigma^2 + w^T w\right)$, that

$$\|A_1\|_2^2 \geq (\sigma^2 + w^T w). \tag{15}$$

But

$$\sigma^2 = \|A\|_2^2 = \|A_1\|_2^2 \geq \sigma^2 + w^T w, \tag{16}$$

and so we must have $w = 0$. An obvious induction argument completes the proof of the theorem.

Exercise 2. *Fill in the details of the above proof.*

Why It Is Important.

The Singular Value Decomposition (SVD) is the most versatile and powerful matrix factorization in numerical linear algebra. It's expensive to compute, but if all else fails the SVD has the best chance of succeeding.

Most applications of the SVD consist of reducing a problem involving A into one involving Σ. Note that since

$$\Sigma = U^T A V \tag{17}$$

Σ is obtained from A by multiplying with two orthogonal matrices, and multiplying with an orthogonal matrix does not amplify errors. So once we know U and V then Σ can be obtained from A in a process that is as well conditioned as it can be.

The Singular Value Decomposition (of square matrices) was first discovered independently by Beltrami in 1873 and Jordan in 1874.

References.

The SVD is discussed in many textbooks on numerical analysis, or numerical linear algebra. The most comprehensive discussion is in the authoritative monograph

- Gene H. Golub and Charles F. van Loan, Matrix Computations, 4th ed., The Johns Hopkins University Press, 2013, ISBN 10: 1-4214-0794-9.

However, the most easily understood first explanation is in

- David Kahaner, Cleve Moler and Stephen Nash, Numerical Methods and Software, Prentice Hall, 1989, ISBN 0-13-627258-4.

The following exercises can help you understand the SVD more thoroughly.

Exercise 3. *Explore how the discussion in these notes has to be modified if $m < n$. One source of problems with underdetermined systems are constrained minimization problems. In that context one is often interested in the* null space *of a matrix, i.e., the space of all vectors that satisfy $Az = 0$. See how to use the SVD to find the null space of A.*

Exercise 4. *Compute the singular value decomposition in the case that $m = 1$ or $n = 1$.*

Exercise 5. *Show that every real $m \times n$ matrix has a singular value decomposition.*

Exercise 6. *Show that the condition number of $A^T A$ is the square of the condition number of A. Comment on the suitability of solving Least Squares Problems via the Normal Equations*

$$A^T A x = A^T b. \tag{18}$$

Exercise 7. *Show that the columns of U are the eigenvectors of AA^T. There are m singular values, but $n \geq m$ eigenvalues of AA^T, so what are the eigenvalues of AA^T?*

Exercise 8. *Ask yourself what happens when A is symmetric. What if it is positive definite?*

Exercise 9. *Investigate the use of the SVD for the solution of eigenvalue problems.*

Exercise 10. *Explore the applicability of the SVD for sparse matrices A.*

Exercise 11. *Using the SVD, express the solution of the Least Squares problem $\|Ax - b\|_2 = \min$ in the form $x = A^+ b$ where A^+ is given in terms of A. A^+ is known as the generalized inverse of A.*

Exercise 12. *Show that*

$$\sigma_1 = \max_{\substack{y \in \mathbb{R}^m \\ x \in \mathbb{R}^n}} \frac{y^T A x}{\|y\|_2 \|x\|_2}. \tag{19}$$

Computing the SVD.

Since the computation of the SVD amounts to the solution of an eigenvalue problem it follows that in general the SVD cannot be computed exactly in a finite number of steps, and so intrinsically one has to use some sort of iteration. The actual computation is involved and sophisticated, for details consult the above mentioned reference by Golub and van Loan. The emphasis in these notes is on what you can actually do with the SVD, once you have it[−4−]. Thus the remainder of these notes lists a sequence of applications of the Singular Value Decomposition.

Some Applications.

Note that the following list in no way is meant to be complete.

Rank Determination.

The rank of a matrix is the maximum number of linearly independent rows or columns. In principle one can compute it by carrying out Gaussian Elimination until it becomes impossible to find a non-zero pivot element by row and column pivoting. The problem of that approach is that because of round-off errors it is extremely difficult to decide when a number is zero. Numbers that should be zero usually aren't because of inexact arithmetic. Since U and V are non-singular the rank of A equals the rank of Σ, and the rank of Σ equals the number of non-zero singular values. In this context, a singular values σ_i is considered zero if

$$\frac{\sigma_i}{\sigma_1} < \tau \tag{20}$$

−4− Software to compute the SVD is available, for example, at

`http://www.netlib.org/`

where τ is a specified tolerance that usually is a small multiple of the round-off unit[−5−]. Another approach is based on looking at the whole set of singular values. Often they decrease gradually and then there is a pronounced jump to very small singular values. If the last singular value before the jump is σ_r then r is the rank of A (and Σ).

Throughout the remainder of this note we will assume that

$$\sigma_1 \geq \sigma_2 \geq \ldots \geq \sigma_r > \sigma_{r+1} = \sigma_{r+2} = \ldots = \sigma_n = 0 \tag{21}$$

and hence

$$\text{rank} A = \text{rank} \Sigma = r. \tag{22}$$

It is of course possible that $r = n$, in which case A has *full rank*.

Computing the Determinant of a Square Matrix. The determinant of an orthogonal matrix is positive or negative 1. The determinant of a square diagonal matrix is the product of its diagonal entries. The determinant of the product of two matrices is the product of the individual determinants. Thus for a square matrix A its determinant is plus or minus the product of the singular values:

$$\det A = \pm \sigma_1 \times \sigma_2 \times \ldots \times \sigma_n. \tag{23}$$

Computing the Condition Number of a Matrix.

Multiplying with an orthogonal matrix does not change the 2-norm of a matrix. The two norm of A is therefore the two norm of Σ which equals σ_1. If A is square and invertible, then its inverse is given by

$$A^{-1} = V \Sigma^{-1} U^T. \tag{24}$$

The matrix Σ^{-1} is diagonal and has the reciprocals of the singular values along the diagonal. Its 2-norm (and that of A^{-1}) is $1/\sigma_n$. Hence,

$$\|A\|_2 \|A^{-1}\|_2 = \frac{\sigma_1}{\sigma_n}. \tag{25}$$

The right hand side of equation (25) makes sense even for rectangular matrices and is usually taken as the definition of the condition number of A even if A is not square. This turns out to be useful beyond being a mere formal generalization.

Note that in the process of computing the condition number we also obtained

$$\|A\|_2 = \sigma_1 \tag{26}$$

−5− The round off unit ϵ, also called the *machine epsilon*, is the smallest number that can be represented on a computer such that the system recognizes $1 + \epsilon$ as being larger than 1. On many systems, including our Unix systems, ϵ equals approximately 2×10^{-16}.

for general matrices A, and

$$\|A^{-1}\| = \frac{1}{\sigma_n} \tag{27}$$

for non-singular square matrices A.

Solving a Linear System.

Let's consider the linear system

$$Ax = b \tag{28}$$

and ask if it has any solutions, and if it does, how many, and what they are. All of these questions can be answered via the SVD. Recalling (5) the system (28) turns into

$$Ax = U\Sigma V^T x = b. \tag{29}$$

Multiplying with U^T gives

$$\Sigma z = c \tag{30}$$

where

$$z = V^T x \quad \text{and} \quad c = U^T b. \tag{31}$$

This is a **diagonal** linear system that can be analyzed easily. Recalling (21) we distinguish three cases:

1. $r = n$ and

$$c_{n+1} = \ldots = c_m = 0. \tag{32}$$

There is a unique solution

$$z_i = \frac{c_i}{\sigma_i}, \quad i = 1, \ldots, n \tag{33}$$

Note that this includes the case $m = n$ where the condition (32) is vacuous.

2. $r < n$ and $c_{r+1} = \ldots = c_m = 0$. In that case

$$z_i = \frac{c_i}{\sigma_i}, \quad i = 1, \ldots, r \tag{34}$$

and z_{r+1} through z_n are arbitrary. There are infinitely many solutions and they form an $n - r$ dimensional affine space[−6−].

3. $r \leq n$ and $c_i \neq 0$ for some $i > r$. In that case the system is inconsistent and there is no solution. Note that this includes the case that $m = n$ (in which case of course the rank r must be less than n for the system to have no solution).

Note that once we have z it is easy to compute

$$x = Vz \qquad (35).$$

−6− An affine space S is a set of vectors $s + v$ where v resides in an ordinary vector space. An example would be a line in the plane, or a plane in three dimensional space. If the line passes through the origin it's a linear subspace, and whether or not it does, it's an affine subspace of the plane.

Also note that all the required transformations involve multiplications with orthogonal matrices, which does not amplify errors.

Solving Least Squares Problems.

Consider the standard Least Squares Problem

$$\|Ax - b\|_2 = \min . \tag{36}$$

The standard approach to this problem is via the QR factorization which we discussed in class. That approach fails if A has a rank less than n. The SVD still works in this case, and once we have it it can of course also be applied in the full rank case. Remembering once again that multiplication with an orthogonal matrix does not alter the 2-norm of a vector, and proceeding similarly as for linear systems we obtain

$$\begin{aligned} \|Ax - b\|_2^2 &= \|U^T(Ax - b)\|_2^2 \\ &= \|U^T AVV^T x - U^T b\|_2^2 \\ &= \|\Sigma z - c\|_2^2 \\ &= \sum_{i=1}^{r} (\sigma_i z_i - c_i)^2 + \sum_{i=r+1}^{m} c_i^2 . \end{aligned} \tag{37}$$

where c and z are defined in (31) and r is defined in (21). There is nothing we can do about the second sum in (37). However, we can render the first sum zero by picking z_i as before in (34). If $r < n$ then we can pick z_{r+1} through z_n arbitrarily. In that case the solution $x = Vz$ of the Least Squares problem is not unique, but the value of Ax is. The usual choice of z in that case is

$$z_{r+1} = z_{r+2} = \ldots = z_n = 0 \tag{38}$$

which gives among all solutions the solution z (and hence x) that itself has the smallest 2-norm.

Data Compression.

It's an easy exercise to see that

$$A = U\Sigma V^T = \sum_{i=1}^{n} \sigma_i u_i v_i^T \tag{39}$$

where the u_i and v_i are the columns of U and V, respectively. Suppose now that A represents an image, or some other kind of data. For example, its entries might be numbers between 0 and 1 that indicate shades of gray. One way to *approximate* A by fewer than mn numbers (and thus compress the image or data) would be to use only the first few terms in the sum on the right of (39), and of course store only the corresponding few left and right singular vectors rather than an $m \times n$ array. The book by Kahaner, Moler and Nash referenced above has an impressive illustration of that technique.