Lecture 5-29

Real symmetric (and more generally complex Hermitian) matrices have so many nice properties that one would like to extend some of them to arbitrary matrices, even rectangular ones. To this end, let A be a complex $m \times n$ matrix and A^* its conjugate transpose. Since the conjugate transpose of a product of matrices is the reverse product of their conjugate transposes, we see that the $n \times n$ matrix $B = A^*A$ is Hermitian; in fact it is also positive semidefinite, since if $v \in \mathbb{C}^n$ then $\bar{v}^T Bv = \bar{v}^T A^*Av = (Av, Av) \in \mathbb{R}, (Av, Av) \geq 0$, where the parentheses denote the Hermitian inner product. If the kernel of A is 0, then B is positive definite. In general, we have seen that B admits a unique positive semidefinite Hermitian square root P. If P is positive definite and thus invertible, set $U = AP^{-1}$, so that $A = UP$; then $U^*U = P^{-1}A^*AP^{-1} = I$, the identity matrix of the appropriate size, since $B = A^*A$ commutes with both its square root and the inverse of this square root. We cannot call the matrix U unitary in general, since it need not even be square, but we can call it the matrix of an isometry, in the sense that $(Uv, Uv) = (v, v)$ whenever Uv is defined. If P is not invertible, then it still defines an invertible linear transformation from its column space to itself; this holds since the column space C of P is the conjugate of its row space R (being obtained from its row space by replacing every coordinate of every vector by its conjugate as a complex number), and the Hermitian product (v, v) of any vector v in R with itself is the dot product of v and its conjugate $\bar{v}$ which is 0 if and only if $v = 0$. Thus no nonzero vector in C has dot product 0 with all of R , and multiplication by P sends to C to itself in a one-to-one and thus onto fashion. There is then a unique isometry mapping any vector $w = Pv \in C$ to Av, where $v \in R$, which we can extend to all of $\mathbb{C}^n$ by decreeing that it send $C^\perp$, the orthogonal complement of C relative to the Hermitian form $(\cdot, \cdot)$, to 0.

Hence in any event we can always write $A = UP$, where P is positive semidefinite and $n \times n$, while we could call U quasi-unitary; it defines an isometry from the column space of P to that of A. This is called the *polar decomposition* of A; in it the matrix P is uniquely determined (as the unique positive semidefinite square root of A^*A, sometimes called the *modulus* of A and denoted $|A|$) but the matrix U is unique if and only if P is positive definite. If $m = n$, so that A is square, then we can take U to be $n \times n$ and unitary in the ordinary sense that $U^* = U^{-1}$. We call $A = UP$ the polar decomposition since it is analogous to writing a complex number $z = a + bi$ as the product $u||z||$ of the norm $||z|| = \sqrt{a^2 + b^2}$ of z and a complex number u of norm 1.

We look at a couple of examples. In all of them we have for simplicity stuck to real matrices and the ordinary dot product, so that our matrices U are orthogonal rather than unitary. If $A = \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}$, then $B = A^*A$ is the 1×1 matrix 3 and $P = \sqrt{3}$. In this case $U = \begin{pmatrix} \frac{1}{\sqrt{3}} \\ \frac{1}{\sqrt{3}} \\ \frac{1}{\sqrt{3}} \end{pmatrix}$ and we have $A = UP, U^*U = 1$. On, the other hand, if $A = (1, 1, 1)$, then $B = \begin{pmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{pmatrix}$, $P = \frac{1}{\sqrt{3}}B$. Here we may take U to be any matrix (a, b, c) with $a + b + c = \sqrt{3}$ and then indeed $A = UP$. The matrix U^*U looks nothing like the 3×3 identity matrix for any choice of a, b, or c, but we observe that any choice of U as above will send $v = \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}$, the unique vector up to scalar multiple in the column space of P to the vector $\sqrt{3} \in \mathbb{C}^1$, whose square length 3 is indeed the same as that of v. Finally, if we let A be our old non-diagonalizable friend $\begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix}$, then it turns out that $U = \frac{1}{\sqrt{5}} \begin{pmatrix} 2 & 1 \\ -1 & 2 \end{pmatrix}, P = \frac{1}{\sqrt{5}} \begin{pmatrix} 2 & 1 \\ 1 & 3 \end{pmatrix}$.

In general the eigenvalues of P, which are the square roots of the eigenvalues of $B = A^*A$, are called the *singular values* of A. If A is real, square, and symmetric, or more generally Hermitian, the its singular values are the same as its eigenvalues, but in general the singular values of A are quite distinct from its eigenvalues; for example, singular values are defined even for nonsquare rectangular matrices A, while eigenvalues are not. Even for square matrices with say rational entries and eigenvalues, their singular values can be irrational. In the example $A = \begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix}$ above, A has 1 as its only eigenvalue, but its singular values are $\frac{\sqrt{5}+1}{2}$ and $\frac{\sqrt{5}-1}{2}$, the unique pair of real numbers with sum equal to the trace $\sqrt{5}$ of P and product equal to its determinant 1.

Combining the polar decomposition with the diagonalization $P = V^{-1}DV$ of any positive semidefinite matrix P by a unitary matrix V, we arrive at the *singular value decomposition* $U\Sigma V$ of any $m \times n$ complex matrix A, usually formulated so that U, V are unitary matrices in the ordinary sense, of sizes $m \times m$ and $n \times n$, respectively, while Σ is an $m \times n$ "diagonal" matrix (all of its entries σ_{ij} with $i \neq j$ are 0; the nonzero entries σ_{ii} are the nonzero singular values of A). In this setup the matrices U and V are not unique, even if A has full rank. Going back to the earlier examples $A = (1,1,1)$ and $(1,1,1)^T$, we find that we may take the 1×1 unitary matrix to be 1 in both cases. The matrix Σ is $(\sqrt{3}, 0, 0)$ for $A = (1,1,1)$ and $(\sqrt{3}, 0, 0)^T$ for $A = (1,1,1)^T$. For $A = (1,1,1)$ we may take the 3×3 unitary matrix to be any orthogonal matrix with first row $(\frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}. \frac{1}{\sqrt{3}})$ for $A = (1,1,1)$ and the transpose of such a matrix in the transposed case. We will give a more careful account of the singular value decomposition next time.