Topics in Linear Algebra

Science Academies' lecture workshop on Mathematical Physics

PSGR Krishnammal College, Coimbatore June 21-23, 2016

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1 Introductory remarks

• The theory of vectors, matrices and linear equations is called linear algebra. It is useful in many classical physics and engineering problems. Linear equations are a first approximation to more complicated and accurate non-linear equations (such as Newton's second law). Near a point of equilibrium we can often linearize the equations of motion to study oscillations: vibrations of a solid or LC oscillations in an electrical circuit.

• Importance of linear algebra in physics is greatly amplified since quantum mechanics is a linear theory.

• Linear algebra is important in analysing experimental data: least squares fitting of data, regression.

• Linear algebra is fun and the basic concepts are not difficult. It has a nice interplay between algebra (calculation) and geometry (visualization). It may also be your first encounter with mathematical abstraction, eg. thinking of spaces of vectors rather than single vectors.

• The basic objects of linear algebra are (spaces of) vectors, linear transformations between them and their representation by matrices.

• Examples of vectors include position $\vec{r}$ and momentum $\vec{p}$ of a particle, electric $\vec{E}(\vec{r},t)$ and magnetic fields at a point, velocity field of a fluid $\vec{v}(\vec{r},t)$. Examples of matrices include inertia tensor I_{ij} of a rigid body, stress tensor (momentum flux density) $S_{ij} = p\delta_{ij} + \rho v_i v_j$ of an ideal fluid, Minkowski metric tensor $\eta_{\mu\nu}$ of space-time in special relativity.

• Matrix multiplication violates the commutative law of multiplication of numbers $AB \neq BA$ in general. Also there can be non-trivial divisors of zero: matrices can satisfy $AB = 0$ with neither A nor B vanishing. Matrix departure from the classical axioms of numbers is as interesting as spherical geometry departure from the axioms of Euclidean geometry.

1.1 Some text books for linear algebra

- C. Lanczos, Applied analysis - chapter 2 on matrices and eigenvalue problems
- C. Lanczos, Linear differential operators, chapter 3 on matrix calculus
- T. M. Apostol, Calculus Vol 2, chapters 1-5
- Gilbert Strang, Introduction to linear algebra
- Gilbert Strang, Linear algebra and its applications
- Courant and Hilbert, Methods of mathematical physics, Vol 1
- Arfken and Weber, Mathematical methods for physicists
- Sheldon Axler, Linear algebra done right
- P.R. Halmos, Finite-dimensional vector spaces
- Erwin Kreyszig, Advanced engineering mathematics
- K T Tang, Mathematical Methods for Engineers and Scientists 1: Complex Analysis, Determinants and Matrices

1.2 A Foretaste: Physical examples of linear equations in matrix form

• Linear algebra deals with systems of linear algebraic equations. One example is the relation of the angular momentum vector to the angular velocity vector of a rigid body: $L = I\Omega$, where

$$I_{ij} = \int \rho(\vec{r}) \left(r^2 \delta_{ij} - r_i r_j \right) d^3 r$$

is the 3×3 real symmetric inertia matrix depending on the mass density ρ of the body. This system of linear equations is expressed in matrix form

$$\begin{pmatrix} L_1 \\ L_2 \\ L_3 \end{pmatrix} = \begin{pmatrix} I_{11} & I_{12} & I_{13} \\ I_{11} & I_{12} & I_{13} \\ I_{11} & I_{12} & I_{13} \end{pmatrix} \begin{pmatrix} \Omega_1 \\ \Omega_2 \\ \Omega_3 \end{pmatrix}. \tag{1}$$

• Many equations of physics and engineering are differential equations (some of which are discussed in the first module of this lecture workshop). Linear algebraic equations often arise from discretizing linear differential equations. Consider for instance the equation for simple harmonic motion $\ddot{x}(t) = -\omega^2 x(t)$. The same differential equation also appears when one separates space and time variables in the wave equation $\partial_t^2 u = c^2 \partial_x^2 u$ for a vibrating string. If $u = T(t)X(x)$, then $\ddot{T}(t) = -\omega^2 T(t)$ and $X''(x) = -k^2 X(x)$ where $\omega = ck$ is a separation constant. In the latter case, this ODE is in fact an eigenvalue problem for the (infinite dimensional) 'matrix' (operator) d^2/dt^2 with $x(t)$ the eigenvector and $-\omega^2$ the eigenvalue (in the case of the harmonic oscillator ω is a fixed constant and we do not interpret the ODE as an eigenvalue problem). It would be nice to see this equation written in terms of matrices and column vectors. To do so we notice that a differential like dx/dt is the limit of a difference quotient $[x(t+\delta t) - x(t)]/\delta t$. By discretizing time we may turn linear differential equations into systems of linear algebraic equations.

• To make this connection explicit, we discretize time and represent $x(t)$ by the column vector whose entries are $x(t_i)$ where t_i are a suitable set of times, say $\delta t(\cdots, -3, -2, -0, 1, 2, 3, \cdots)$ where δt is a small time-step. We write it as the transpose of a row vector to save space

$$x(t) \approx \begin{pmatrix} \cdots & x(-2\delta t) & x(-\delta t) & x(0) & x(\delta t) & x(2\delta t) & \cdots \end{pmatrix}^t. \tag{2}$$

Approximating $\dot{x}(t) \approx (x(t+\delta t) - x(t))/\delta t$ by the *forward* difference, we have for instance $\dot{x}(0) = (x(\delta t) - x(0))/\delta t$ etc. Thus the entries of the column vector for $\dot{x}$ are

$$\frac{dx(t)}{dt} \approx \frac{1}{\delta t} \begin{pmatrix} \vdots \\ x(-\delta t) - x(-2\delta t) \\ x(0) - x(-\delta t) \\ x(\delta t) - x(0) \\ x(2\delta t) - x(\delta t) \\ x(3\delta t) - x(2\delta t) \\ \vdots \end{pmatrix} = \begin{pmatrix} \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ \dots & -1 & 1 & 0 & 0 & 0 & \dots \\ \dots & 0 & -1 & 1 & 0 & 0 & \dots \\ \dots & 0 & 0 & -1 & 1 & 0 & \dots \\ \dots & 0 & 0 & 0 & -1 & 1 & \dots \\ \dots & 0 & 0 & 0 & 0 & -1 & \dots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \end{pmatrix} \begin{pmatrix} \vdots \\ x(-2\delta t) \\ x(-\delta t) \\ x(0) \\ x(\delta t) \\ x(2\delta t) \\ \vdots \end{pmatrix} \tag{3}$$

From this we see that d/dt may be represented by a matrix with -1s along the diagonal, $+1$s along the first super diagonal and zeros elsewhere. Other discretizations are possible. For instance, we could use the *backward* difference $\dot{x}(t) \approx (x(t) - x(t-\delta t))/\delta t$, in which case the corresponding matrix would have 1s along the diagonal and -1s along the first sub-diagonal. The more symmetrical centered-difference $\dot{x} \approx (x(t+\delta t) - x(t-\delta t))/2\delta t$ leads to a tri-diagonal matrix with zeros along the diagonal and ± 1 along the first super(sub) diagonal. All these formulae tend to the derivative $\dot{x}$ in the limit as $\delta t \to 0$.

• A convenient discretization for the second derivative is

$$\ddot{x} \approx \frac{1}{\delta t}\left(\frac{x(t+\delta t) - x(t)}{\delta t} - \frac{x(t) - x(t-\delta t)}{\delta t}\right) = \frac{x(t+\delta t) - 2x(t) + x(t-\delta t)}{(\delta t)^2}. \tag{4}$$

Then we may represent the operator d^2/dt^2 in this basis by a tri-diagonal real symmetric matrix, a few of whose 'middle' rows and columns are

$$\frac{d^2}{dt^2} \approx \frac{1}{(\delta t)^2}\begin{pmatrix} \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ \dots & -2 & 1 & 0 & 0 & 0 & \dots \\ \dots & 1 & -2 & 1 & 0 & 0 & \dots \\ \dots & 0 & 1 & -2 & 1 & 0 & \dots \\ \dots & 0 & 0 & 1 & -2 & 1 & \dots \\ \dots & 0 & 0 & 0 & 1 & -2 & \dots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \end{pmatrix} \quad \text{where} \quad x(t) \approx \begin{pmatrix} \vdots \\ x(-2\delta t) \\ x(-\delta t) \\ x(0) \\ x(\delta t) \\ x(2\delta t) \\ \vdots \end{pmatrix} \tag{5}$$

Thus we have approximated the linear differential equation $\ddot{x} = -\omega^2 x$ by an infinite system of linear algebraic equations expressed in terms of column vectors and matrices:

$$\frac{1}{(\delta t)^2}\begin{pmatrix} \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ \dots & -2 & 1 & 0 & 0 & 0 & \dots \\ \dots & 1 & -2 & 1 & 0 & 0 & \dots \\ \dots & 0 & 1 & -2 & 1 & 0 & \dots \\ \dots & 0 & 0 & 1 & -2 & 1 & \dots \\ \dots & 0 & 0 & 0 & 1 & -2 & \dots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \end{pmatrix}\begin{pmatrix} \vdots \\ x(-2\delta t) \\ x(-\delta t) \\ x(0) \\ x(\delta t) \\ x(2\delta t) \\ \vdots \end{pmatrix} = -\omega^2 \begin{pmatrix} \vdots \\ x(-2\delta t) \\ x(-\delta t) \\ x(0) \\ x(\delta t) \\ x(2\delta t) \\ \vdots \end{pmatrix}. \tag{6}$$

This is called an eigenvalue problem, $-\omega^2$ is the eigenvalue, and a non-zero column vector $x(t)$ satisfying this equation is called an eigenvector of the matrix. We will introduce and study eigenvalue problems in more detail. $x(t)$ clearly has infinitely many components, and the tri-diagonal matrix representing d^2/dt^2 has infinitely many entries. We say that d^2/dt^2 is an operator on an infinite dimensional vector space. To understand these terms and concepts we begin with some elementary notions and definitions.

2 Vector spaces

• Often our first examples of vectors are vectors in the plane or in three dimensional space. These are geometrically viewed as directed line segments from the origin to a point. If Cartesian coordinates are used, then the coordinates (x, y) or (x, y, z) of the tip of the vector are called the components of the vector $\vec{v} = (x, y, z)$ (we will often omit the vector sign and speak of the vector v). On the plane, $\hat{x} = (1, 0)$ and $\hat{y} = (0, 1)$ are called the unit vectors in the corresponding directions.

2.1 Linear combinations and (in)dependence

• Given a collection of vectors $v_1, v_2, \cdots, v_n$, a linear combination is a weighted sum $a_1 v_1 + a_2 v_2 + \cdots a_n v_n$, where a_i are numbers (real or complex). For example, $3\hat{x} + 2\hat{y}$ is a linear combination of these two unit vectors.

• Vectors are linearly dependent if there is a non-trivial linear combination of them that vanishes. i.e. the vectors satisfy a linear relation. For example $\hat{x}$ and $3\hat{x}$ are linearly dependent since they satisfy the linear relation $3(\hat{x}) - 3\hat{x} = 0$. More formally, $v_1, v_2, \cdots, v_n$ are linearly dependent if $\sum_{i=1}^{n} a_i v_i = 0$ for some real numbers a_i not all zero.

• On the other hand, there is no non-trivial linear combination of $u = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$ and $v = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}$ that vanishes. We say that u, v are linearly independent.

• Definition: $v_1, v_2, \cdots, v_n$ are linearly independent if: $a_1 v_1 + a_2 v_2 + \cdots a_n v_n = 0$ implies that $a_1 = a_2 = a_3 = \cdots = a_n = 0$.

2.2 Definition and basic examples of vector spaces

1. The basic operation defining a vector space is that of taking linear combinations of vectors $av + bw$. a, b are called scalars and v, w vectors.
2. A vector space is a space of vectors that is closed under linear combinations with scalar coefficients.
3. The multiplication by scalars distributes over addition of vectors $a(v + w) = av + aw$.
4. The scalars a, b that we can multiply a vector by are either real or complex numbers and give rise to a real or complex vector space. More generally, they can come from a field.
5. Examples of vector spaces: $R^2, R^3, R, C^2, R^n, C^n$
6. Non-examples: the following are not closed under linear combinations
    - A line not passing through the origin.
    - A half plane or quadrant or the punctured plane.
    - Unit vectors in R^2
7. So a vector space is also called a linear space, it is in a sense flat rather than curved.

2.3 Linear span of vectors

• Given vectors v, w, say in R^3, we can form all possible linear combinations with real or complex coefficients, $\{av + bw | a, b \in \mathbf{R} \text{ or } \mathbf{C}\}$. This is their (real or complex linear) span. For example, $3v - w$ is a linear combination. Unless otherwise specified, we will use real coefficients.

• $span(v, w)$ is a two dimensional plane provided v and w were linearly independent. It is a vector space by itself.

• Eg $a\hat{x} + b\hat{y}$ is the span of the unit vector in the x and y directions. Geometrically, we go a units in the horizontal direction and b units in the vertical direction.

• For example, the span of the unit vector $\hat{x}$ is the x-axis while the span of $(1,0,0)$ and $(0,1,0)$ is the whole $x-y$ plane R^2 contained inside R^3

2.4 Subspace

• A subspace W of a vector space V is a subset $W \subseteq V$ that forms a vector space by itself under the same operations that make V a vector space.

• The span of any set of vectors from a vector space forms a vector space. It is called the subspace spanned by them.

• e.g., Any line or plane through the origin is a subspace of R^3. So is the point $(0,0,0)$.

• On the other hand, notice that $u = (1,0,0), v = (0,1,0), w = (1,2,0)$ span the same $x-y$ plane. There is a redundancy here, we don't need three vectors to span the plane, two will do.

• In other words, $w = (1,2,0)$ already lies in the span of $u = (1,0,0)$ and $v = (0,1,0)$, since $w - u - 2v = 0$.

• We say that u, v, w are linearly dependent if there is a non-trivial linear combination that vanishes.

• On the other hand, u and v are linearly independent and they span the plane.

• We say u, v are a basis for the plane.

2.5 Basis

• A basis for a vector space is a linearly independent collection of vectors $\{v_1, v_2, \cdots, v_n\}$ which span the space.

• $\hat{x}, \hat{y}$ is the standard basis for R^2, but $3\hat{x} + 2\hat{y}, \hat{y}$ is also a basis. Notice that bases have the same number of vectors (cardinality).

• The standard basis for R^n is the Cartesian one $(e_i)_j = \delta_{ij}$

$$e_1 = \begin{pmatrix} 1 \\ 0 \\ 0 \\ \vdots \\ 0 \end{pmatrix}; \; e_2 = \begin{pmatrix} 0 \\ 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix}; \; \cdots; e_n = \begin{pmatrix} 0 \\ 0 \\ 0 \\ \vdots \\ 1 \end{pmatrix}. \tag{7}$$

• Every vector can be *uniquely* written as a linear combination of basis vectors $x = x_i v_i$. We say that we have decomposed x into its components x_i in the basis. Proof: Suppose x has two *different* decompositions $x = x_i v_i$ and $x = x_i' v_i$, then $0 = x - x = (x_i - x_i')v_i$. But then we have a linear combination of basis vectors that vanish, which is not possible since v_i were linearly independent. So $x_i = x_i'$.

2.6 Dimension

• The dimension of a vector space is the cardinality of any basis. Equivalently, it is the maximal number of linearly independent vectors in the space.

• The dimension d of a subspace of an n-dimensional space must satisfy $0 \leq d \leq n$. The difference $n - d$ is called the co-dimension of the subspace.

• The dimension of C^n as a complex vector space is n. But it is also a real vector space of dimension $2n$

• Note that the dimension of a vector space should not be confused with the number of vectors in the space. The number of vectors is 1 for the trivial vector space and infinite otherwise.

• $\{(0)\}$ is not a basis for the 'trivial' vector space consisting of the zero vector alone. This is because the zero vector does not form a linearly independent set, it satisfies the equation $5(0) = 0$ for instance. The dimension of the trivial vector space is zero.

2.7 More examples of vector spaces

• The space consisting of just the zero vector is a 0-dimensional space, the trivial vector space.

• Consider the set of 2×2 *real matrices*. We can add matrices and multiply them by real numbers and the results are again 2×2 real matrices. So this is a real vector space $M_2(R)$. More generally we have the real vector space $M_n(R)$. The dimension of $M_2(R)$ is 4. What is a basis? Note that if we consider the same set of 2×2 real matrices, it fails to be a complex vector space. Multiplication by an imaginary number takes us out of the set.

• The vector space of solutions of a *homogeneous linear differential equation*: For example consider the differential equation for the motion of a free particle on a line $x(t) \in R$ $m\frac{\partial^2 x}{\partial t^2} = 0$. If $x(t)$ and $y(t)$ are solutions, then so is any real linear combination of them. This is a two dimensional real vector space, spanned by 1 and t. Acting on this space of solutions, we may think of $m\frac{\partial^2}{\partial t^2}$ as the 2×2 zero matrix.

• Vector space spanned by the words in an alphabet: Given the English alphabet of 26 letters, we can form all words (with or without meaning) by stringing letters together. Now consider all real linear combinations of these words, such as the vectors

$$\begin{aligned} v &= 10 \text{ a} + 23 \text{ cat} - \pi \text{ xyz} + \text{dog} \\ w &= \text{pig} - 7 \text{ xyz} + 4\text{dog} \end{aligned} \tag{8}$$

Then $v + w = 10 \text{ a} + 23 \text{ cat} - (7 + \pi) \text{ xyz} + 5 \text{ dog} + \text{pig} - 7 \text{ xyz}$ This is a real vector space. But it is infinite dimensional since there are an infinite number of (largely meaningless!) words. A basis consists of all possible words.

• We see that vector spaces are often specified either by giving a basis or as the solution space to a system of linear equations. A geometric example of a vector space is the space vectors tangent to a curve or surface at a point. For example, the tangent space to the sphere at the north pole is a two dimensional real vector space.

3 Linear transformations between vector spaces and matrices

• A linear transformation from domain vector space D to target vector space T is a linear map taking vectors in D and producing vectors in T:

$$L : D \to T, \qquad L(au + bv) = aL(u) + bL(v) \tag{9}$$

• You can either form linear combinations before applying L or afterwards, the result is the same. Importantly, $L(0) = 0$.

3.1 Matrix of a linear map

• Consider a linear transformation $L : R^n \to R^m$, suppose we take the standard Cartesian bases for R^n and R^m. L is determined by how it acts on the basis vectors e_i of R^n. Here $e_1 = (1\,0\,0\cdots)^t$ etc. If $v = v_i e_i$ is a linear combination of basis vectors, then $L(v_i e_i) = v_i L(e_i)$. So suppose $L(e_i) = f_i$ where $f_i \in R^m$ are the images of e_i. We view the f_i as m-component column vectors. Then the matrix representation of L in these bases is the $n \times m$ matrix whose columns are the images f_i of the basis vectors e_i. $L = (f_1\, f_2\, f_3 \cdots f_n)$.

• Example. Consider a rotation R by 90 degrees counter clockwise on the $x - y$ plane. Why is it linear? In the standard basis for R^2, the images of the basis vectors are $R\hat{x} = \hat{y} = (0,1)^t$ and $R\hat{y} = -\hat{x} = (-1,0)^t$. Thus $R = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$.

• The matrix of a linear transformation will generally be different in different bases. Only very special linear maps have the same matrix in all bases, these are multiples of the identity map $L(e_i) = \lambda e_i$, which are represented by λ times the identity matrix I.

• Example: The projection $P : R^2 \to R^2$ that projects every geometric vector to its horizontal component. Check that this is a linear transformation. Here the domain and target are the same vector space, so we can use a single basis. If f_1 and f_2 are the standard cartesian basis vectors in the horizontal and vertical directions, then $Pf_1 = f_1$ and $Pf_2 = 0$. In the f-basis, the columns of the matrix representation of P are the images of f_1 and f_2, so

$$f_1 = \begin{pmatrix} 1 \\ 0 \end{pmatrix}_f, \quad f_2 = \begin{pmatrix} 0 \\ 1 \end{pmatrix}_f, \quad P_f = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}. \tag{10}$$

Since P is diagonal in the f-basis, we say that the f-basis is an eigenbasis for P. f_1, f_2 are eigenvectors of P with eigenvalues 1 and 0.

• Notice that $P_f^2 = P_f$, this is common to all projection matrices: projecting a vector for a second time does not produce anything new.

• But we are not obliged to work in the standard cartesian basis. So let us pick another basis consisting of $e_1 = f_1$ and $e_2 = f_1 + f_2$. So geometrically, e_1 is the standard cartesian horizontal basis vector, but e_2 is a vector that points north-east. In the f-basis we have

$$e_1 = \begin{pmatrix} 1 \\ 0 \end{pmatrix}_f, \quad e_2 = \begin{pmatrix} 1 \\ 1 \end{pmatrix}_f \tag{11}$$

But $\{e_1, e_2\}$ are also a basis in their own right. So we can also write e_1, e_2 in the e-basis

$$e_1 = \begin{pmatrix} 1 \\ 0 \end{pmatrix}_e, \quad e_2 = \begin{pmatrix} 0 \\ 1 \end{pmatrix}_e \tag{12}$$

So we see that the same geometric vector may have different representations in different bases! Now the matrix of the projection P in the e-basis is the matrix whose columns are the images of e_1 and e_2 in the e-basis. Since $Pe_1 = e_1$ and $Pe_2 = e_1$, we have

$$P_e = \begin{pmatrix} 1 & 1 \\ 0 & 0 \end{pmatrix} \tag{13}$$

P is not diagonal in the e-basis, so the e_i are not an eigenbasis for P. Nevertheless, the e-basis is a legitimate basis to use.

• Moreover, even in the e-basis, we see that $P_e^2 = P_e$

• We see that the same linear transformation P can have different matrix representations in different bases. However, P_e and P_f are related by a *change of basis*. First observe that the two bases are related by $e_1 = f_1, \quad e_2 = f_1 + f_2$ which may be written in matrix form as

$$e \equiv \begin{pmatrix} \vec{e}_1 \\ \vec{e}_2 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 1 & 1 \end{pmatrix} \begin{pmatrix} \vec{f}_1 \\ \vec{f}_2 \end{pmatrix} \equiv S^t \begin{pmatrix} \vec{f}_1 \\ \vec{f}_2 \end{pmatrix} \quad \text{where} \quad S = \begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix} \tag{14}$$

In short $e = S^t f$. Calling it S^t is a matter of convenience so that the columns (rather than rows) of S are the components of e_i in the f-basis. S is called a change of basis. Notice that S is invertible, which is guaranteed since its columns form a basis and so are linearly independent.

• Now we can state the change of basis formula for a matrix: $P_e = S^{-1}\ P_f\ S$, which can be checked in our case

$$S^{-1}\ P_f\ S = \begin{pmatrix} 1 & -1 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix} = \begin{pmatrix} 1 & 1 \\ 0 & 0 \end{pmatrix} = P_e \tag{15}$$

3.2 Matrix multiplication

• Composition of linear transformations corresponds to matrix multiplication.

• An $m \times n$ matrix is a rectangular array of numbers (real or complex) with m rows and n columns. If $m = n$ we have a square matrix. If $m = n = 1$ the matrix reduces to a number (scalar). A $1 \times n$ matrix is a row vector. An $m \times 1$ matrix is a column vector.

• Matrix multiplication in components $\sum_{k=1}^{n} A_{ik} B_{kj} = C_{ij}$. Summation convention: repeated indices are summed except when indicated otherwise. Sometimes we write A^i_k for A_{ik}, with row superscript and column subscript. Then $A^i_k B^k_j = C^i_j$.

• Matrix multiplication is associative, can put the brackets anywhere $A(BC) = (AB)C \equiv ABC$. To see this, work in components and remember that multiplication of real/complex numbers is associative

$$[A(BC)]_{il} = A_{ij}(BC)_{jl} = A_{ij} B_{jk} C_{kl} = [(AB)C]_{il}. \tag{16}$$

• Matrix multiplication distributes over addition $A(B + C) = AB + AC$. Addition of matrices is commutative $A + B = B + A$, we just add the corresponding entries.

• The zero matrix is the one whose entries are all $0's$. $A + 0 = A$ and $0A = 0$ for every matrix, and $0v = 0$ for every vector.

• **Outer product** of a column vector with a row vector gives a matrix: This is just a special case of matrix multiplication of $A_{m\times 1}$ with $B_{1\times n}$ to give a matrix $C_{m\times n}$. For example

$$\begin{pmatrix} x \\ y \end{pmatrix} \begin{pmatrix} z & w \end{pmatrix} = \begin{pmatrix} xz & xw \\ yz & yw \end{pmatrix} \tag{17}$$

• Example that shows a product of non-zero matrices can be zero

$$\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix} \tag{18}$$

• Multiplication of matrices is in general not commutative, i.e. AB need not equal BA. For example, check this for

$$A = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad B = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{19}$$

In this case you will find that $AB = -BA$. But this is not so in general, as the following example indicates

$$A = \begin{pmatrix} 1 & 2 \\ 3 & 4 \end{pmatrix}, \quad B = \begin{pmatrix} 2 & 3 \\ -1 & -2 \end{pmatrix} \Rightarrow AB = \begin{pmatrix} 0 & -1 \\ -2 & 3 \end{pmatrix}, \quad BA = \begin{pmatrix} 11 & 16 \\ -7 & -8 \end{pmatrix}. \tag{20}$$

• A way of looking at matrix vector multiplication: $\begin{pmatrix} a & b \\ c & d \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = x \begin{pmatrix} a \\ c \end{pmatrix} + y \begin{pmatrix} b \\ d \end{pmatrix}$ as linear combinations of columns: $x\times$ first column plus $y\times$ second column.

• Av multiplication of a column vector by a matrix from the left is a new column vector. It is a linear combination (specified by the components of v), of the columns of A

$$\begin{pmatrix} | & | & . & . & | \\ c_1 & c_2 & . & . & c_n \\ | & | & . & . & | \end{pmatrix} \begin{pmatrix} v_1 \\ v_2 \\ . \\ . \\ v_n \end{pmatrix} = v_1 \begin{pmatrix} | \\ c_1 \\ | \end{pmatrix} + v_2 \begin{pmatrix} | \\ c_2 \\ | \end{pmatrix} + \cdots v_n \begin{pmatrix} | \\ c_n \\ | \end{pmatrix} \tag{21}$$

• Row picture of multiplication of a row vector from right by a matrix xA. The result is a linear combination of the rows of A, i.e. a new row vector.

$$\begin{pmatrix} x_1 & x_2 & . & . & x_m \end{pmatrix} \begin{pmatrix} \text{row}_1 \\ \text{row}_2 \\ . \\ . \\ \text{row}_m \end{pmatrix} = x_1(\text{row}_1) + x_2(\text{row}_2) + \cdots + x_m(\text{row}_\text{m}) \tag{22}$$

3.3 Inverse of a square matrix, kernel or null space and rank

• A square matrix maps n-component column vectors in the domain to n-component column vectors in the target. The inverse of A (when it exists) must go in the opposite direction.

• The problem of inverting a matrix A is related to the problem of solving $Ax = b$ and expressing the answer as $x = Lb$. But for this to be the case, we need $LA = I$. This motivates the definitions that follow.

• If A has a left inverse $LA = I$ and a right inverse $AR = I$, then they must be the same by associativity (we can move brackets around)

$$(LA)R = L(AR) \quad \Rightarrow \quad IR = LI \quad \Rightarrow \quad R = L = A^{-1} \tag{23}$$

• An $n \times n$ square matrix is defined to be invertible if there is a matrix A^{-1} satisfying $A^{-1}A = AA^{-1} = I$. If not, A is called singular.

• In terms of maps, invertibility implies that A and A^{-1} must be 1-1. Moreover, the image of A must be the domain of A^{-1}, and the image of A^{-1} must equal the domain of A.

• When the inverse exists, it is unique by associativity. Suppose A has two inverses B and C, then by definition of inverse,

$$AB = BA = I, \qquad CA = AC = I. \tag{24}$$

Using associativity, $(CA)B = C(AB)$ but this simplifies to $B = C$.

• A real number is a 1×1 matrix. It is invertible as long as it is not zero. Its inverse is the reciprocal.

• A 2×2 matrix $A = (ab|cd)$ is invertible iff the *determinant* $ad - bc \neq 0$. Its inverse is

$$A^{-1} = \begin{pmatrix} a & b \\ c & d \end{pmatrix}^{-1} = \frac{1}{ad - bc} \begin{pmatrix} d & -b \\ -c & a \end{pmatrix} \tag{25}$$

• A matrix is invertible iff $A_{n \times n}$ does not annihilate any non-zero vector. Vectors annihilated by A are called its zero-modes and they form a vector space called its kernel $\ker(A)$ or null space $N(A)$.

• Indeed, if A is invertible, then $Ax = 0$ implies $x = A^{-1}0 = 0$, so A has a trivial kernel.

• For the converse note that if A has trivial kernel, then A is $1-1$. Indeed, if A were not $1-1$, then there would be distinct non-zero vectors x, y such that $Ax = Ay$ or $A(x - y) = 0$ but then $x - y$ would lie $\ker(A)$. On the other hand, if $\ker(A)$ is trivial, then the columns of A are linearly independent[1]. So the image of A is the whole of the target space of n-component vectors. So if A has trivial kernel, then A is both $1-1$ and onto and therefore invertible.

• The point about invertibility of A is that it *guarantees unique* solutions to the $n \times n$ systems $Ax = b$ and $yA = c$ for *any* column n-vector b and any row n-vector c: $x = A^{-1}b$ and $y = cA^{-1}$. But in practice inverting a matrix is not an efficient way of solving a particular system of equations (i.e. for a specific b or c). Elimination is better.

• So square A is invertible iff the columns (or rows) of A are linearly independent.

• Example: Inverse of a diagonal matrix $A = \text{diag}(\lambda_1, \cdots, \lambda_n)$ is again diagonal with entries given by the reciprocals, $A^{-1} = \text{diag}(\lambda_1^{-1}, \cdots, \lambda_n^{-1})$.

[1] Indeed $Av = v_1c_1 + v_2c_2 + \cdots v_nc_n$ is a linear combination of the columns of A. So if the columns are linearly independent, this vanishes only if $v_i \equiv 0$.

• Example of a singular matrix $A = \begin{pmatrix} 1 & 1 \\ 0 & 0 \end{pmatrix}$. This matrix annihilates the vector $x = \begin{pmatrix} -1 \\ 1 \end{pmatrix}$. It has a row of zeros. It has only one pivot. Its determinant vanishes. And finally, we can't solve $Ax = \begin{pmatrix} 1 \\ 2 \end{pmatrix}$ for instance. What are the only $b's$ for which we can solve $Ax = b$?

• $A = \begin{pmatrix} 1 & 2 \\ 2 & 4 \end{pmatrix}$ is also singular. The second row is twice the first. Check the other equivalent properties.

• The inverse of an elimination matrix is easily found. Suppose A subtracts twice the first row from the second row of a 2×2 matrix. Then its inverse must add twice the first row to the second.

$$A = \begin{pmatrix} 1 & 0 \\ -2 & 1 \end{pmatrix} \quad \Rightarrow \quad A^{-1} = \begin{pmatrix} 1 & 0 \\ 2 & 1 \end{pmatrix} \tag{26}$$

• Eg: $A = \begin{pmatrix} -1 & 2 & 0 \\ 3 & -4 & 2 \\ 6 & -3 & 9 \end{pmatrix}$. This matrix has a non-trivial kernel. Notice that the third column is twice the first added to the second. So any vector of the form $c \begin{pmatrix} 2 \\ 1 \\ -1 \end{pmatrix}$ is annihilated by A. So it is not invertible.

• The inverse of a product is the product of inverses in the reversed order, when they exist. To see why, draw a picture of the maps.

$$(AB)^{-1} = B^{-1}A^{-1} \quad \text{since} \quad B^{-1}A^{-1}AB = I \tag{27}$$

• The sum of invertible matrices may not be invertible, e.g. $I - I = 0$ is not invertible.

• There is a formula for the inverse, $A^{-1} = C(A)^t / \det A$. Here we assume familiarity with the determinant and the matrix of cofactors $C(A)$. The transpose is defined shortly.

• Remark: If A is an $n \times n$ matrix, we can express its inverse (when it exists) using its minimal polynomial, which is a polynomial of minimal degree $p(x) = p_0 + p_1 x + \cdots p_k x^k$ such that $p(A) = 0$. A matrix is invertible iff $p_0 \neq 0$. In that case, $A^{-1} = -p_0^{-1}(p_1 + p_2 A + \cdots p_n A^{n-1})$. $p(x)$ may have degree less than n and need not be the same as the characteristic polynomial, though it is always a factor of the characteristic polynomial $\det(A - xI) = 0$.

• The **rank** of a matrix is the number of linearly independent columns or rows. An invertible $n \times n$ matrix has maximal rank n.

3.4 Transpose

• Transpose of an $m \times n$ matrix is the $n \times m$ matrix whose rows are the columns of A (in the same order).

• In components, $(A^t)_{ij} = A_{ji}$

• Transpose of a column vector is a row vector.

• $(A^t)^t = A$ and $(AB)^t = B^t A^t$ and we also have $(x^t A y)^t = y^t A^t x$.

• A square matrix which is its own transpose $A^t = A$ is called symmetric. Real symmetric matrices are a particularly nice class of matrices and appear in many physics and geometric problems. They appear in quadratic forms defining the kinetic energy of a free particle or a system of free particles. Real symmetric matrices behave a lot like real numbers.

• The operations of transposition and inversion commute $(A^{-1})^t = (A^t)^{-1}$. Proof: Suppose A is an invertible square matrix (i.e., has two-sided inverse $AA^{-1} = A^{-1}A = I$). Then A^t is also invertible and $(A^t)^{-1} = (A^{-1})^t$. To see this just take the transpose of $A^{-1}A = AA^{-1} = I$ to get $A^t(A^{-1})^t = (A^{-1})^t A^t = I$. But this is saying that $(A^{-1})^t$ is the inverse of A^t. In other words $(A^{-1})^t = (A^t)^{-1}$.

• The inverse of a symmetric invertible matrix $A^t = A$ is again symmetric. Suppose $B = A^{-1}$

$$AB = BA = I \Rightarrow B^t A^t = A^t B^t = I \Rightarrow B^t A = AB^t = I \quad (28)$$

So B^t is also the inverse of A and by uniqueness of the inverse, $B^t = B$.

3.5 Trace of a square matrix

• **The trace of a matrix is the sum of its diagonal entries in any basis** $\text{tr}\, A = A_{ii}$. $\text{tr}\, A$ is also the sum of its eigenvalues.

• **The trace is cyclic:** $\text{tr}\, AB = \text{tr}\, BA$, since $\text{tr}\, AB = A_{ij}B_{ji} = B_{ji}A_{ij} = \text{tr}\, AB$. It follows that $\text{tr}\, ABC = \text{tr}\, CAB = \text{tr}\, BCA$.

• We anticipate the **basis independence of the trace** under similarity transformations: $\text{tr}\, S^{-1}AS = \text{tr}\, SS^{-1}A = \text{tr}\, A$. In particular the trace is **invariant under orthogonal and unitary transformations** $\text{tr}\, Q^tAQ = \text{tr}\, A$, $\text{tr}\, A = \text{tr}\, U^\dagger AU$.

4 Inner product, norm and orthogonality

• The standard inner product (dot product) on R^n is $x \cdot y = (x, y) = x^t y = \sum_i x_i y_i$. Here we think of x, y as a column vectors, their inner product is a scalar (real number). The inner product is symmetric $(x, y) = (y, x)$ and linear in each entry: $(ax, y) = a(x, y)$ and $(x + y, z) = (x, z) + (y, z)$. A vector space with an inner product is also called a Hilbert space.

• The norm or length of a vector $||x||$ is the square-root of its inner product with itself $||x|| = (x^t x)^{1/2}$. Then norm is the usual Euclidean length of the vector since $||x||^2 = x^t x = x_1^2 + x_2^2 + \cdots x_n^2 \geq 0$. The only vector with zero norm is the zero vector.

• Suppose x and y are a pair of vectors at right angles. The hypotenuse of the right triangle formed by them has length $||x + y||$, so $||x + y||^2 = ||x||^2 + ||y||^2$. The LHS-RHS must vanish,

$$||x + y||^2 - ||x||^2 - ||y||^2 = (x + y)^t (x + y) - x^t x - y^t y = x^t y + y^t x = 2(x, y) = 0 \quad (29)$$

So if a pair of vectors are orthogonal (i.e. at right angles), their inner product vanishes $(x, y) = 0$. The converse is also true, $a^2 + b^2 = c^2$ implies that a, b, c are the lengths of the sides of a right triangle. This follows from the cosine formula in trigonometry: $a^2 + b^2 - 2ab\cos\theta = c^2$, where a, b, c are the lengths of the sides of a triangle. So a pair of vectors are orthogonal iff their inner product vanishes.

• Cauchy-Schwarz Inequality: For a pair of n-vectors x, y, the Cauchy-Schwarz inequality is

$$|(x,y)|^2 \leq (x,x)(y,y) \quad \text{or} \quad |(x,y)| \leq ||x||\ ||y|| \tag{30}$$

It says that the cosine of the angle between a pair of vectors is of magnitude ≤ 1:

$$\cos\theta = \frac{(x,y)}{||x||\ ||y||} \tag{31}$$

• The triangle inequality states that $||x+y|| \leq ||x|| + ||y||$. It says that the length of a side of a triangle is always $\leq$ the sum of the lengths of the other two sides. Draw a picture of this. We have equality precisely if $x = \lambda y$ (i.e. they are collinear).

• For complex vectors in C^n, the standard (hermitian) inner product is $(z,w) = \bar{z}^t w = z^\dagger w$, where $\bar{z}$ denotes the complex conjugate vector.

• For a complex number $z = x+iy$ with real x, y, the complex conjugate $\bar{z} = z^* = x - iy$. The absolute value of a complex number is its length in the complex plane $|z| = \sqrt{|\bar{z}z|} = \sqrt{x^2+y^2}$. The notation $\bar{z}$ is more common in the mathematics literature while z^* is more common in physics to denote the complex conjugate.

• The complex conjugate transpose, $z^\dagger$ is called the (Hermitian) adjoint of the vector z. For complex vectors, the hermitian adjoint plays the same role as the transpose does for real vectors.

• This is the appropriate inner product since it ensures that $(z,z) = ||z||^2 = z^\dagger z = |z_1|^2 + \cdots |z_n|^2$ is real and non-negative and so its positive square-root $(z^\dagger z)^{1/2}$ may be interpreted as the length of the vector z.

• The hermitian inner product is not symmetric but satisfies $(z,w)^* = (w,z)$.

• A pair of vectors are orthogonal if their inner product vanishes $z^\dagger w = 0$.

• In the language of quantum mechanics, a vector is a possible state of a system and a (hermitian) matrix is an observable. Expectation value of a matrix observable A in the state x is defined as the complex number $x^\dagger A x / x^\dagger x$.

4.1 Orthonormal bases

• A basis $\{q_i\}_{i=1}^n$ for a vector (sub)space is orthogonal if the basis vectors are mutually orthogonal, $q_i \perp q_j$ or $q_i^t q_j = 0$ for $i \neq j$.

• In addition it is convenient to normalize the basis vectors to have unit length, $||q_i|| = 1$. Then we say the basis q_i is orthonormal or o.n.

• Example, the standard cartesian $x-y$ basis is o.n. But so is any rotated version of it. The columns of Q and Q' below are both o.n. bases for R^2

$$Q = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \qquad Q' = \begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix} \tag{32}$$

• The basis $(1,0,0)$ and $(0,1,0)$ is an orthonormal basis for the $x-y$ plane contained in R^3. In this case Q is a rectangular 3×2 matrix,

$$Q = \begin{pmatrix} 1 & 0 \\ 0 & 1 \\ 0 & 0 \end{pmatrix} \tag{33}$$

yet it satisfies $Q^t Q = I_{2\times 2}$. Note that $QQ^t \neq I$, in fact it is a projection matrix!

• But if $Q_{n\times n}$ is a square matrix, then $Q^t Q = I$ implies that Q has a left inverse. Does it have a right inverse? Being a basis, we know that the columns of Q are linearly independent. Being square, the rows must also be linearly independent as the rank is n. But if the rows are linearly independent, it means the rows span the domain or equivalently, $c = yQ$ has a unique solution for any c. This means Q has a right inverse. By the equality of left and right inverses, we conclude that $Q^{-1} = Q^t$ and that $QQ^t = Q^t Q = I$. Such a matrix is called an orthogonal matrix.

4.2 Hilbert spaces and Dirac bra-ket notation

• A finite dimensional Hilbert space $\mathcal{H}$ is a finite dimensional vector space with an inner product (u, v) that is linear in v and anti-linear in u satisfying

$$(u, v) = (v, u)^* \quad \text{and} \quad (u, u) > 0, \quad \text{for} \quad u \neq 0 \tag{34}$$

• We will work with the example C^n with the standard inner product $(z, w) = z^\dagger w$. Notice that $(z, w) = (w, z)^*$. Moreover, for scalars a, b, $(az, w) = \bar{a}(z, w)$ while $(z, bw) = b(z, w)$. Finally, $(z, w + u) = (z, w) + (z, u)$. These properties ensure linearity in the second entry and anti-linearity in the first.

• Dirac notation: If we think of $V = C^n$ as made of column vectors, we denote the column vector v as the ket-vector $|v\rangle$. The space of ket-vectors form the vector space V. Similarly the n-component row vectors with complex entries are called the bra-vectors $\langle v|$. Moreover, $\langle v| = |v\rangle^\dagger$ and $\langle v|^\dagger = |v\rangle$ are adjoints of each other. For example

$$|v\rangle = \begin{pmatrix} 1 \\ i \\ -2i + 3 \end{pmatrix}, \quad \langle v| = |v\rangle^\dagger = \begin{pmatrix} 1 & -i & 2i + 3 \end{pmatrix} \tag{35}$$

The space of bra-vectors form a so-called dual space V^* to V. V and V^* are isomorphic vector spaces. Indeed any row vector $\langle w|$ defines a linear function $f_{\langle w|}$ on V, given by

$$f_{\langle w|}(|v\rangle) = \langle w|v\rangle \tag{36}$$

The dual space V^* is defined as the space of linear functions on V. $\langle w|v\rangle$ is called the pairing between the dual spaces.

• If $|v\rangle = \sum_i v_i |\phi_i\rangle$ is expressed as a linear combination of $|\phi_i\rangle$, then $\langle v| = |v\rangle^\dagger = \sum_i \langle \phi_i| v^*$.

• If e_i are a basis, $v \in \mathcal{H}$ a vector and $A : \mathcal{H} \to \mathcal{H}$ a linear transformation, then we can write $Ae_j = \sum_i A_{ij} e_i$ and $v = \sum_j v_j e_j$ and $Av = \sum_j v_j A e_j = \sum_{ij} v_j A_{ij} e_i = \sum_{ij} (A_{ij} v_j) e_i$. In other words $(Av)_i = A_{ij} v_j$. Now let us assume that e_i are an orthonormal basis, so $\langle e_i|e_j\rangle = \delta_{ij}$. Then we have

$$A|e_j\rangle = A_{ij}|e_i\rangle \quad \Rightarrow \quad \langle e_k|A|e_j\rangle = \sum_i A_{ij}\langle e_k|e_i\rangle = \sum_i A_{ij}\delta_{ki} = A_{kj} \tag{37}$$

We conclude that $A_{ij} = \langle e_i|A|e_j\rangle$ in any orthonormal basis $\{e_i\}$. Similarly, in an orthonormal basis, $|v\rangle = \sum_i v_i |e_i\rangle$ implies that $v_j = \langle e_j|v\rangle$. Thus the components of a vector or a matrix are easy to find in an o.n. basis using the inner product.

• In a finite dimensional Hilbert space, we have seen that any vector can be decomposed in an o.n. basis as $|v\rangle = \sum_i \langle e_i|v\rangle |e_i\rangle$ or rearranging, $|v\rangle = \sum_i |e_i\rangle\langle e_i|v\rangle$. So we see that the linear transformation $\sum_i |e_i\rangle\langle e_i|$ takes every vector to itself, in other words, it must be the identity transformation, which is represented by the identity matrix in any basis. So

$$\sum_i |e_i\rangle\langle e_i| = I \tag{38}$$

This is called the completeness relation or property. We see that it is the sum of outer products of the orthonormal basis vectors $e_i e_i^\dagger = I$. It says that the sum of the projections to the one-dimensional subspaces spanned by the o.n. basis vectors e_i is the identity. We say that e_i are a complete o.n. basis.

• For example, $\begin{pmatrix} 1 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 1 \end{pmatrix}$ form a complete o.n. basis for R^2. The completeness relation is satisfied:

$$\begin{pmatrix} 1 \\ 0 \end{pmatrix} (\, 1 \quad 0 \,) + \begin{pmatrix} 0 \\ 1 \end{pmatrix} (\, 0 \quad 1 \,) = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \tag{39}$$

• For a finite dimensional Hilbert space, every o.n. basis is complete. More generally, a sequence of vectors $u_i \in \mathcal{H}$ is complete if there is no non-zero vector in $\mathcal{H}$ that is orthogonal to all of them.

• Similarly, for the bra-vectors, completeness of the o.n. basis e_i allows us to write

$$\langle v| = \sum_i \langle v|e_i\rangle\langle e_i| = \sum_i v_i^* \langle e_i| \tag{40}$$

• Let us see some more uses of the completeness relation of an orthonormal basis

$$\langle v|w\rangle = \sum_i \langle v|e_i\rangle\langle e_i|w\rangle = \sum_i v_i^* w_i \tag{41}$$

We say that we have inserted the identity between $\langle v|$ and $|w\rangle$.

• $\langle v|v\rangle = ||v||^2 = \sum_i \langle v|e_i\rangle\langle e_i|v\rangle = \sum_i \langle v|e_i\rangle\langle v|e_i\rangle^* = \sum_i |\langle v|e_i\rangle|^2$. This expresses the norm^2 of v as the sum of the absolute squares of its components in a complete o.n. basis.

• Note that for brevity, sometimes the basis-kets are denoted $|i\rangle$ instead of $|e_i\rangle$.

• Recover the formula for matrix multiplication: $(AB)_{ij} = \langle i|AB|j\rangle = \sum_k \langle i|A|k\rangle\langle k|B|j\rangle = \sum_k A_{ik}B_{kj}$. The completeness relation says $I = \sum_i |i\rangle\langle i| = \sum_i P_i$ where $P_i = |i\rangle\langle i|$ (no sum on i) is the projection to the subspace spanned by $|i\rangle$.

• $P_i P_j = |i\rangle\langle i|j\rangle\langle j| = |i\rangle\delta_{ij}\langle j| = \delta_{ij}P_j$ (no sum on i or j). This says for instance that projections to orthogonal subspaces is zero $P_1P_2 = 0$ while $P_1P_1 = P_1$.

• A hermitian matrix $H^\dagger = H$ is also called self-adjoint. $(H^\dagger)_{ij} = H_{ij}$ can be written as $\langle i|H^\dagger|j\rangle = \langle i|H|j\rangle$. Now notice that $\langle j|H|i\rangle^* = \langle j|H|i\rangle^\dagger = \langle i|H^\dagger|j\rangle$. So the condition of hermiticity can be expressed

$$\langle i|H|j\rangle = \langle j|H|i\rangle^* \tag{42}$$

5 Consistency of $Ax = b$. Particular and general solutions

• Consider the system of inhomogeneous linear equations $Ax = b$ for an $n \times n$ matrix A and n-component column vector b. We have n equations in n unknowns (the components of the column vector x). This is called an even determined system[2]. b is called the inhomogeneity or source. If $b = 0$ the system is homogeneous. Though it is called an even determined system, it may have zero, one or infinitely many solutions depending on the nature of A and b.

• First b and A must satisfy a compatibility condition, without which there are no solutions. The condition simply states that b must lie in the image of A, i.e., b bust be a linear combination of the columns of A. A more useful form of the condition is obtained by taking the transpose of the equation $x^t A^t = b^t$. Now taking the inner product with an arbitrary vector y we get $x^t A^t y = b^t y = (b, y)$. Thus a necessary consistency condition is that $b^t y$ must be zero whenever y is annihilated by A^t. In other words, b must be orthogonal to the null space of A^t. Henceforth, we suppose the compatibility condition $b \cdot N(A^t) = 0$ is satisfied.

• To find the nature of solutions to $Ax = b$ we notice that if x and x' are both solutions, then $A(x - x') = 0$. In other words two solutions differ by a solution of the homogeneous equation or equivalently $x - x'$ must lie in the kernel $N(A)$. Now suppose x_p is one 'particular' solution of $Ax = b$. Then the general solution is given by $x_p + x_h$ where $x_h \in N(A)$ is any homogeneous solution. Thus the solution space to $Ax = b$ has dimension equal to that of the kernel of A. An interesting special case is when $N(A)$ is trivial, consisting only of the zero vector. In this case A is invertible and we have a unique solution $x = A^{-1}b$. Moreover, in this case A^t is also invertible and $N(A^t)$ is trivial so that the consistency condition $b \cdot N(A^t)$ is automatically satisfied.

• A particularly important special case is the homogeneous equation $Ax = 0$. $x = 0$ is always a solution, the trivial solution. If A is invertible, then there are no non-trivial solutions. A non-trivial solution exists iff $\det A \neq 0$. In general, the solution space is just the kernel or null space of A.

6 Operators on inner-product spaces

• An *inner product space* is a vector space V with an inner product (x, y) (which is a scalar, real or complex) for $x, y \in V$. The inner product on a real vector space must be symmetric $[(x, y) = (y, x)]$ and bilinear $[(ax + by, z) = a(x, z) + b(y, z)]$. For example, R^n with the standard dot product $(x, y) = x^t y$ is an inner product space. Inner product spaces are also called *Hilbert spaces* and are the arena for geometric discussions concerning lengths and angles as well as for quantum dynamics.

• Suppose $A : U \to U$ is a linear transformation from the inner product space U to itself, then we call A an **operator on the inner product space** U. This concept also applies to $A : U \to V$.

• **Dirac Bra-Ket notation:** Suppose e_i are a basis for a vector space, say R^n. Think of these as column vectors. Dirac's notation for them is $|e_i\rangle$. Indeed any column vector x is called a ket-vector, and may be written as a linear combination $|x\rangle = \sum_{i=1}^n x_i |e_i\rangle$. On the other

[2]More generally we could have m equations in n unknowns. In this case x is an n-component column vector, A an $m \times n$ matrix and b an m-component column vector.

hand, the basis of row vectors e_i^t are denoted $\langle e_i|$. Any row vector y is a linear combination $\langle y| = \sum_i y_i \langle e_i|$.

• Moreover, the inner product is written as $(x,y) = \langle x|y\rangle = \sum_{i,j} x_i y_j \langle e_i|e_j\rangle$. If e_i are an orthonormal basis, then $\langle e_i|e_j\rangle = \delta_{ij}$, and $\langle x|y\rangle = \sum_i x_i y_i$.

• The **matrix elements** A_{ij} of a linear transformation $A : V \to V$ in the basis e_i is given by

$$A_{ij} = e_i^t A e_j = (e_i, Ae_j) = \langle e_i|A|e_j\rangle \tag{43}$$

To see this note that Ae_j is the j^{th} column of A and $e_i^t A$ is the i^{th} row of A or equivalently, the i^{th} column of A^t. Combining these, $e_i^t A e_j$ is the entry in the i^{th} row and j^{th} column. Alternatively, write e_j in the e-basis as the column vector with zeros everywhere except for a 1 in the j^{th} slot and similarly e_i^t as the row vector with a 1 in the i^{th} slot and zeros elsewhere and perform the matrix multiplication.

• More generally, A could be rectangular. Suppose $A : U \to V$, then the matrix element A_{ij} in the e_j basis for U and f_i basis for V is given by $A_{ij} = f_i^t A e_j = (f_i, Ae_j) = \langle f_i|A|e_j\rangle$.

6.1 Orthogonal transformations

• A **rotation** of the plane about the origin is a linear transformation that **preserves distances and angles**. A **reflection** about a line through the origin also **preserves lengths and angles of vectors**. Orthogonal transformations generalize this concept to other dimensions. Recall that the inner product is used to define lengths of vectors as well as angles between vectors.

• An **orthogonal transformation** on a real inner product space is one which **preserves the inner product**, i.e. $(u,v) = (Qu, Qv)$ for all u, v. It is called orthogonal because it is represented by an orthogonal matrix, as we will see. Transformations that preserve inner products are also called isometries.

• In particular, an orthogonal transformation $u \to Qu$ preserves the length of u: $(u,u) = ||u||^2 = (Qu,Qu) = ||Qu||^2$ and the angle between u and v: $\frac{(u,v)}{||u||||v||} = \frac{(Qu,Qv)}{||Qu||||Qv||}$. For the standard inner product $(u,v) = u^t v$, we have $u^t v = u^t Q^t Q v$. Since this is true for all u and v, it follows that $Q^t Q = I$. In more detail, take u and v to be any orthonormal basis $e_i^t e_j = \delta_{ij}$, then $u^t v = u^t Q^t Q v$ becomes $e_i^t Q^t Q e_j = e_i^t e_j = \delta_{ij}$. This merely says that the matrix elements of $Q^t Q$, $(Q^t Q)_{ij} = e_i^t Q^t Q e_j$ are the same as the matrix elements of the unit matrix.

• So an orthogonal matrix is an $n \times n$ matrix that satisfies $Q^t Q = I$. In other words, the columns of Q are orthonormal. So the left inverse of Q is Q^t. But we showed earlier that if the columns of Q are orthonormal, then the right inverse is also Q^t. In other words $QQ^t = Q^t Q = I$. This means the rows of Q are also orthonormal.

• The inverse and transpose of an orthogonal matrix are also orthogonal. Check that the product of two orthogonal matrices is also orthogonal.

• The identity matrix and $-I$ are obviously orthogonal. The reflection in the x axis in R^2 is orthogonal

$$Q = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{44}$$

• A 2×2 real matrix $\begin{pmatrix} a & b \\ c & d \end{pmatrix}$ is orthogonal provided the rows are orthonormal: $a^2+b^2=c^2+d^2=1$ and $ac+bd=0$. These conditions can be 'solved' in terms of trigonometric functions. 2×2 orthogonal matrices are either **rotations** by θ

$$Q = \begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix} \tag{45}$$

or **rotations by θ composed with a reflection** $(x,y)\to(x,-y)$

$$Q = \begin{pmatrix} \cos\theta & \sin\theta \\ \sin\theta & -\cos\theta \end{pmatrix}. \tag{46}$$

• Permutation matrices are matrices obtained from permutations of the columns (rows) of the identity matrix. But permuting the columns (rows) does not change the fact that the columns (rows) of I are orthonormal. So **permutation matrices are orthogonal**

$$Q_{(132)} = \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}. \tag{47}$$

So the inverse of a permutation matrix is just its transpose $Q_{132}^t Q_{132} = I$.

6.2 Unitary transformations

• A **unitary transformation preserves the inner product on a complex vector space** $(z,w)=(Uz,Uw)$ for all z,w. For the standard hermitian inner product on C^n, $(z,w)=z^\dagger w$ this becomes $z^\dagger w = (Uz,Uw) = z^\dagger U^\dagger U w$. Repeating the steps used for orthogonal matrices, unitary matrices are those square matrices that satisfy

$$U^\dagger U = U U^\dagger = I \tag{48}$$

Here the hermitian adjoint of any matrix or vector is the complex conjugate transposed: $A^\dagger = (A^t)^*$. Notice that $(z,Aw) = z^\dagger A w = (A^\dagger z)^\dagger w = (A^\dagger z, w)$ where we used $(A^\dagger)^\dagger = A$.

• For a general inner product space the adjoint $A^\dagger$ of a matrix A is defined through its matrix elements using the above relation $(A^\dagger z, w) \equiv (z, Aw)$.

• We notice that the **inverse of a unitary matrix U is its adjoint $U^\dagger$**.

• All real orthogonal matrices are automatically unitary, since complex conjugation has no effect.

• A 2×2 complex matrix $\begin{pmatrix} a & b \\ c & d \end{pmatrix}$ is unitary provided $|a|^2+|b|^2=|c|^2+|d|^2=1$, $a\bar{c}+b\bar{d}=0$.

• Define the matrix exponential as the matrix $e^{Ax} = \sum_{n=0}^\infty \frac{A^n x^n}{n!}$. The sum is absolutely convergent for any square matrix and defines e^{Ax}. We can use it to find more unitary matrices, the exponential of any anti-hermitian matrix is unitary.

• Example: $\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$ is the first Pauli matrix, it is hermitian. It turns out that $U = e^{i\sigma_1 x}$ is a unitary matrix for any real x. To see this, use the formula for the matrix exponential to show that $U = e^{i\sigma_1 x} = I\cos x + i\sigma_1 \sin x$. It follows that $U^\dagger = I\cos x - i\sigma_1\sin x$ and that $U^\dagger U = UU^\dagger = I$.

6.3 Orthogonal projection and projection matrices

• Projections are an important class of matrices, not least because the **density matrix of a pure state of a quantum system is a projection matrix**.

• **Orthogonal projection onto a line through the origin:** A line through the origin is just a 1-d vector space spanned by a vector a. We seek to project a vector v onto the span of a. Let us call the projection $Pv = a\xi$, where ξ is a scalar, since Pv must be a multiple of a. Then the orthogonality of the projection means that the difference between v and its projection Pv, i.e. the **error vector** $e = v - Pv$ **must be perpendicular to** a

$$e \perp a \quad \Rightarrow \quad a^t e = 0 \Rightarrow a^t(v - Pv) = 0 \quad \Rightarrow \quad a^t v = \xi a^t a \quad \Rightarrow \quad \xi = \frac{a^t v}{a^t a}. \tag{49}$$

• So $Pv = a\xi = \frac{aa^t}{a^t a} v$.

• Another way to find the projection $P_a v$ is to observe that $Pv = \xi a$ is the **vector along** a **that is closest to** v. So ξ must be chosen so that the error vector $e = v - Pv$ has minimal length.

$$||e||^2 = (v - \xi a)^t (v - \xi a) = v^t v - 2\xi a^t v + \xi^2 a^t a \Rightarrow \frac{\partial ||e||^2}{\partial \xi} = -2a^t v + 2\xi a^t a = 0 \Rightarrow \xi = \frac{a^t v}{a^t a}. \tag{50}$$

• Projection map $v \mapsto Pv$ is a linear transformation, since it is linear in v. The matrix of the projection onto the subspace spanned by a is

$$P_a = \frac{aa^t}{a^t a} \quad \text{or} \quad P_{ij} = \frac{a_i a_j}{\sum_k a_k a_k} \tag{51}$$

• The product of a column vector by a row vector with the same number n of components is called the outer product, it is an $n \times n$ matrix. So P_a is the **outer product** of a with itself **divided by the inner product** of a with itself. Notice that $P_a a = a$. Also, if $v \perp a$ ($v^t a = 0$), then $P_a v = 0$.

• It is easy to check that P_a satisfies the following two properties: it is **symmetric** $P^t = P$ **and squares to itself** $P^2 = P$. We will see that more general projections also satisfy these properties and they can be taken as the defining properties of projections. Caution: $P^t = P$ is true only in orthonormal bases.

• Notice that $I - P_a$ also satisfies these conditions. It is the **projection onto the orthogonal complement** of a. Indeed, it is just the error vector $(I - P_a)v = v - P_a v$, which we know to be orthogonal to $\vec{a}$.

• For example, the projection matrix onto the line spanned by the unit column vector $a = (1, 0, 0)$ is

$$P_a = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \tag{52}$$

Notice that $\text{tr}\, P_a = 1$ is its rank, P_a has one independent column or row. **In general, the trace of a projection is the dimension of the space to which it projects.**

• However, **not all rank-1 matrices are projections**. A rank-1 matrix can always be written as an outer product $A = uv^t$. Multiplying by columns we see that uv^t is the matrix whose columns are $(v_1 u, v_2 u, \cdots, v_n u)$, so it has only one linearly independent column. Conversely, any matrix with only one linearly independent column is of this form. Only if u, v point in the same direction and have reciprocal lengths is the rank one matrix uv^t a projection.

• Consider another example, projection onto $a = \begin{pmatrix} 1 \\ 2 \end{pmatrix}$

$$P_a = \frac{1}{5}\begin{pmatrix} 1 & 2 \\ 2 & 4 \end{pmatrix}, \qquad \text{tr } P_a = 1 \tag{53}$$

• Since $P_a = P_{\lambda a}$ we see that P_a **only depends on the subspace spanned by** a.

• If $a \perp b$, i.e. $b^t a = 0$, then $P_a P_b = P_b P_a = 0$ as can be seen from the formula. **Projections to orthogonal directions commute**.

• **Projection to orthonormal basis vectors:** A virtue of orthonormal bases is that it is very easy to find the projection onto a basis vector in an orthonormal basis. If $\vec{x} = \sum_i x_i \vec{e}_i$ where $\vec{e}_i$ are an o.n. basis, then $P_{e_i} x = x_i \vec{e}_i$ (no sum on i) where $x_i = (x, e_i)$ are the components. To see this use the above formula and orthonormality $\vec{e}_i^t \vec{e}_j = \delta_{ij}$

$$P_{e_i} x = \frac{e_i e_i^t}{e_i^t e_i} x = e_i e_i^t x = e_i x_i \qquad \text{(no sum on } i) \tag{54}$$

In particular, any vector can be expanded in an orthonormal basis $\vec{e}_i$ as $a = \sum_i P_{e_i} a$

6.4 Gram-Schmidt orthogonalization

• We have seen that orthonormal bases $q_i^T q_j = \delta_{ij}$ are very convenient, The components of any vector in an orthonormal basis are just its inner products with the basis vectors

$$x = x_i q_i \Rightarrow x_i = (q_i, x) \tag{55}$$

• So given any basis, it is useful to convert it into an orthonormal basis. This is what the **Gram-Schmidt** procedure of successive orthogonalization does. It begins with linearly independent vectors $a_1, a_2 \cdots a_n$ which may be regarded as the columns of A. From them, it produces an orthonormal basis for the column space $C(A)$, $q_1, q_2, \cdots q_n$.

• Suppose first that the a_i are orthogonal but not necessarily of length 1. Then we can get an orthonormal basis by defining $q_i = \frac{a_i}{||a_i||}$. So the key step is to get an orthogonal basis of vectors.

• To start with, let $q_1 = a_1/||a_1||$. The next vector is a_2, but it may not be orthogonal to a_1, so we subtract out its projection on a_1, and then normalize the result. We continue this way:

$$\begin{aligned} \tilde{q}_1 &= a_1, & q_1 &= \tilde{q}_1/||q_1|| \\ \tilde{q}_2 &= a_2 - P_{q_1} a_2, & q_2 &= \tilde{q}_2/||q_2|| \\ \tilde{q}_3 &= a_3 - P_{q_1} a_3 - P_{q_2} a_3, & q_3 &= \tilde{q}_3/||q_3|| \\ &\vdots & & \\ \tilde{q}_n &= (1 - P_{q_1} - P_{q_2} - \cdots - P_{q_{n-1}}) a_{n-1}, & q_n &= \tilde{q}_n/||q_n|| \end{aligned} \tag{56}$$

• By construction, for each r, q_r is orthogonal to all the q's before it, and it is normalized. So we have an orthonormal system of vectors which may be assembled as the columns of an orthogonal matrix $Q = (q_1 q_2 \cdots q_n)$, $Q^T Q = I$

• But we also see the triangular character of the construction. a_1 is along q_1, a_2 is a combination of q_1 and q_2, a_r is a combination of $q_1 \cdots q_r$ etc. But precisely which combinations? To find out, we just reap the benefit of our construction. Since q_i are an orthonormal basis, the components of any vector in this basis are just the inner products:

$$\begin{aligned}
a_1 &= (q_1, a_1) q_1 \\
a_2 &= (q_1, a_2) q_1 + (q_2, a_2) q_2 \\
a_2 &= (q_1, a_3) q_1 + (q_2, a_3) q_2 + (q_3, a_3) q_3 \\
&\vdots \\
a_n &= (q_1, a_n) q_1 + (q_2, a_n) q_2 + \cdots + (q_n, a_n) q_n
\end{aligned} \tag{57}$$

• In matrix form this is $A = QR$

$$\begin{pmatrix} a_1 & a_2 & \cdots & a_n \end{pmatrix} = \begin{pmatrix} q_1 & q_2 & \cdots & q_n \end{pmatrix} \begin{pmatrix} q_1^T a_1 & q_1^T a_2 & \cdots & q_1^T a_n \\ 0 & q_2^T a_2 & \cdots & q_2^T a_n \\ 0 & 0 & \cdots & \cdots \\ 0 & 0 & \cdots & q_n^2 a_n \end{pmatrix} \tag{58}$$

• As an example, let us find the orthonormal basis arising from and the corresponding QR decomposition

$$a_1 = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, a_2 = \begin{pmatrix} 1 \\ 2 \\ 0 \end{pmatrix}, a_3 = \begin{pmatrix} 1 \\ 2 \\ 3 \end{pmatrix} \tag{59}$$

In this case you can guess the answer easily.

• Apply the Gram-Schmidt procedure to the following basis for R^3

$$a_1 = \begin{pmatrix} 1 \\ -1 \\ 0 \end{pmatrix}, a_2 = \begin{pmatrix} 2 \\ 0 \\ -2 \end{pmatrix}, a_3 = \begin{pmatrix} 3 \\ -3 \\ 3 \end{pmatrix} \tag{60}$$

• Use the QR decomposition to invert A.

• 2 dimensional example

$$a_1 = \begin{pmatrix} \sin\theta \\ \cos\theta \end{pmatrix}, a_2 = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \tag{61}$$

• Consider the vector space of real polynomials in one variable $-1 \leq x \leq 1$ with the inner product $(f, g) \int_{-1}^{1} f(x) g(x) dx$. A basis is given by the monomials $1, x, x^2, x^3, \ldots$. However the basis is not orthogonal or even normalized, for example $(1, 1) = 2$. Use the Gram-Schmidt procedure to convert it to an orthonormal basis. The corresponding polynomials are the Legendre polynomials.

6.5 Invariance of matrix equations under orthogonal/unitary and general linear changes of basis

• Consider the matrix equation $Ax = b$. Since both x and b are vectors, they transform in the same way under an orthogonal transformation, say $x = Q\bar{x}$ and $b = Q\bar{b}$. Thus

$$AQ\bar{x} = Q\bar{b} \quad \Rightarrow \quad Q^t AQ\bar{x} = \bar{b} \tag{62}$$

• Thus the equation takes the same form in the new reference frame if we let $\bar{A} = Q^t AQ$. This is the transformation rule for a matrix under an orthonormal change of basis.

• It follows that $\bar{A} + \bar{B} = Q^t(A + B)Q$ and $\bar{A}\bar{B} = Q^t ABQ$. So any polynomial (algebraic function) in matrices transforms in the same way as a single matrix.

$$F(\bar{A}, \bar{B}, \cdots, \bar{P}) = Q^t F(A, B, \cdots, P)Q \tag{63}$$

• So if we have an algebraic relation among matrices $F(A, B, \cdots P) = 0$ then we have the same algebraic relation among the orthogonally transformed matrices

$$F(\bar{A}, \bar{B}, \cdots, \bar{P}) = 0. \tag{64}$$

• Thus we have the invariance of matrix equations under orthogonal transformations.

• Moreover, the inverse of an (invertible) matrix transforms in the same way $\bar{A}^{-1} = Q^t A^{-1} Q$.

• Furthermore, the transpose of a matrix transforms in the same way: $\bar{A}^t = Q^t A^t Q$. So any algebraic matrix equation involving matrices, their inverses and their transposes is invariant under orthogonal transformations.

• If we replace orthogonal by unitary and transpose by adjoint, all of the above continues to hold. So a matrix that is hermitian in one o.n. frame is hermitian in every other o.n. basis for C^n.

• While components of vectors and matrices generally transform as above, some special vectors and matrices, have the same components in every o.n. frame. These are the zero vector and multiples of the identity matrix.

• The angle between two vectors, length of a vector and inner product of a pair of vectors are also invariant under orthogonal and unitary transformations as discussed earlier. The trace and determinant of a matrix are also orthogonally and unitarily invariant, as discussed shortly.

• Algebraic equations in matrices (not involving the transpose) are also invariant under general linear transformations $\bar{A} = S^{-1}AS$, where S is invertible but not necessarily orthogonal or unitary. General linear transformations are also called similarity transformations.

7 Diagonalization of square matrices: eigenvalues and eigenvectors

• For an $n \times n$ matrix, the domain and target space are both R^n or both C^n and may be identified. So $x \mapsto Ax$ transforms $x \in C^n$ to another vector in C^n. The vectors that behave in the simplest manner are those sent to a multiple of themselves. If $Ax = \lambda x$ then A does not change the direction of x. The equation $Ax = \lambda x$ is called the **eigenvalue problem** for A. A **non-zero solution** x **is called an eigenvector** corresponding to the **eigenvalue or characteristic value** λ.

• The **subspace spanned by an eigenvector** x is called an **invariant subspace** under A. This is a particularly useful feature if we want to apply A again, for then $A^2x = \lambda^2 x$, $A^3x = \lambda^3 x, \cdots$. An **eigenvector does not 'mix' with other vectors** under application of A. This is very useful in solving time-evolution problems. Eg systems of differential equations $\frac{\partial u}{\partial t} = Au$, where we need to apply A repeatedly to evolve $u(t)$ forward in time.

• The scalars $\lambda_1, \lambda_2, \cdots, \lambda_n$ for which the eigenvalue problem can be solved non-trivially are called the eigenvalues and the corresponding **non-zero vectors** $x_1, x_2, \cdots x_n$ are the **eigenvectors or principal axes**. The zero vector $x = 0$ is not considered an eigenvector of any matrix, since it trivially solves $Ax = \lambda x$ for any λ.

• Eigen-vector is a German word meaning own-vector, the eigenvectors of a matrix A are characteristic or special vectors associated to A, they are like its private property.

• Note that if x is an eigenvector of A with eigenvalue λ, $Ax = \lambda x$, then so is any non-zero multiple, $A(cx) = \lambda(cx)$. So **eigenvectors are defined up to an arbitrary normalization (scale) factor**. Often, it is convenient to normalize eigenvectors to have length one, $||x|| = 1$.

• Consider $Ax = \lambda x$ which is the **homogeneous system** $(A - \lambda I)x = 0$. We know that a non-trivial solution (eigenvector) exists iff $\det(A - \lambda I) = 0$.

• So the eigenvalues λ_i are precisely the solutions of $\det(A - \lambda I) = 0$.

$$\det(A - \lambda I) = \det \begin{pmatrix} a_{11} - \lambda & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} - \lambda & \alpha_{23} & \cdots \\ \vdots & \vdots & \vdots & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nn-\lambda} \end{pmatrix} = 0 \quad (65)$$

• This is an n^{th} **order polynomial equation** in λ. It is called the **characteristic equation**.

• For example, the characteristic equation of the real symmetric matrix $A = \begin{pmatrix} 1 & 2 \\ 2 & 4 \end{pmatrix}$ is

$$\det \begin{pmatrix} 1 - \lambda & 2 \\ 2 & 4 - \lambda \end{pmatrix} = (1 - \lambda)(4 - \lambda) - 4 = \lambda^2 - 5\lambda = \lambda(\lambda - 5) = 0 \quad (66)$$

The eigenvalues are $\lambda = 0, 5$ and the corresponding eigenvectors are $\begin{pmatrix} 2 \\ -1 \end{pmatrix}$ and $\begin{pmatrix} 1 \\ 2 \end{pmatrix}$. Notice that the eigenvalues are real, we will see that had to be the case because A is symmetric. The determinant is $1 \times 4 - 2 \times 2 = 0$ which is the same as the product of eigenvalues, 5×0. Notice that the trace is $1 + 4 = 5$ which is the same as the sum of eigenvalues.

• The characteristic polynomial $\det(A - \lambda I)$ has n complex roots. These **roots** $\lambda_1, \lambda_2, \cdots, \lambda_n$ **are the** n **eigenvalues** of an $n \times n$ matrix. Generically, they are distinct. But it may happen that some of the eigenvalues coincide. **Repeated roots** should be **counted with (algebraic) multiplicity**.

• So the characteristic polynomial may be written as

$$\det(A - \lambda I) = (\lambda_1 - \lambda)(\lambda_2 - \lambda) \cdots (\lambda_n - \lambda) \quad (67)$$

• Actually, it is convenient to multiply by $(-1)^n$ so that the polynomial is monic, i.e. coefficient of λ^n is 1. Expanding out the product, the characteristic equation may be written as

$$(-1)^n \det(A - \lambda I) = \lambda^n + c_{n-1}\lambda^{n-1} + c_{n-2}\lambda^{n-2} + \cdots c_1\lambda + c_0 = 0 \quad (68)$$

• Setting $\lambda = 0$ we see that the constant term is the **determinant** upto a possible sign and this may also be identified with the **product of eigenvalues**

$$(-1)^n \det A = c_0; \qquad \det A = \lambda_1 \lambda_2 \cdots \lambda_n \tag{69}$$

• Moreover $-c_{n-1}$, the coefficient of $-\lambda^{n-1}$ is the **sum of the eigenvalues** $\lambda_1 + \lambda_2 + \cdots + \lambda_n$. It turns out that this is the **trace** of A.

• The eigenvalues of A^t are the same as the eigenvalues of A. This is because $\det(A^t - \lambda I) = \det(A - \lambda I)$. So A and A^t have the same characteristic polynomial.

• To any given eigenvalue λ_1, there is a solution to the eigenvalue problem $A\vec{u}_1 = \lambda_1 \vec{u}_1$, giving the eigenvector $\vec{u}_1 = \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix}$. In summary,

$$\begin{array}{rl} \text{eigenvalues :} & \lambda_1,\ \lambda_2,\ \cdots,\ \lambda_n \\ \text{eigenvectors :} & \vec{u}_1,\ \vec{u}_2,\ \cdots,\ \vec{u}_n \end{array} \tag{70}$$

• For example, for the 3×3 identity matrix, the roots of the characteristic equation $(\lambda - 1)^3 = 0$ are $\lambda = 1, 1, 1$, and we would say that 1 is an eigenvalue with (algebraic) multiplicity three. We also say that 1 is an eigenvalue with degeneracy 3. If eigenvalue λ has multiplicity 1 we say it is a non-degenerate eigenvalue.

• The identity matrix $I_{n\times n}$, satisfies $Ix = x$ for every vector. So every non-zero vector is an eigenvector. The characteristic equation is $(\lambda - 1)^n = 0$, so the only eigenvalue is 1, with an algebraic multiplicity n. Moreover, since every non-zero vector is an eigenvector, there are n-linearly independent eigenvectors corresponding the the eigenvalue 1.

• The **space spanned by the eigenvectors corresponding to eigenvalue λ is called the λ-eigenspace** of A. This is because it is closed under linear combinations and forms a vector space $Ax = \lambda x, Ay = \lambda y \Rightarrow A(cx + dy) = \lambda(cx + dy)$.

• For the identity matrix $I_{n\times n}$, the 1-eigenspace is the whole of R^n.

• The **dimension of the λ-eigenspace is called the geometric multiplicity** of eigenvalue λ. It is always $\leq$ algebraic multiplicity. For the identity matrix, the algebraic and geometric multiplicities of eigenvalue 1 are both equal to n.

• A matrix is **deficient** if the **geometric multiplicity of some eigenvalue is strictly less than its algebraic multiplicity**. This means it is **lacking in eigenvectors**. Analysis of such matrices is more involved. Fortunately, the matrices we encounter often in basic physics ((anti)symmetric, orthogonal, (anti)hermitian and unitary) are not deficient.

• The eigenvectors of non-deficient $n \times n$ matrices span the whole n-dimensional vector space.

• An **example of a deficient matrix** is

$$N = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \quad \Rightarrow \quad \det(N - \lambda I) = \lambda^2 = 0 \quad \Rightarrow \quad \lambda_1 = 0, \quad \lambda_2 = 0 \tag{71}$$

The eigenvectors are then the non-trivial solutions of $\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = 0$. So there is only one independent eigenvector $\begin{pmatrix} 1 \\ 0 \end{pmatrix}$. So the 0-eigenspace is 1-dimensional, though the eigenvalue 0 has algebraic multiplicity two. In this case, the eigenvectors do not span the whole of R^2.

• On the other hand, the **eigenvectors corresponding to a pair of distinct eigenvalues are always linearly independent**.

• Proof: So we are given $Ax = \lambda x$ and $Ay = \mu y$, with $\lambda \neq \mu$ and eigenvectors $x, y \neq 0$. Now suppose x, y were linearly dependent, i.e. $cx + dy = 0$ with $c, d \neq 0$. We will arrive at a contradiction. Applying A,

$$cAx + dAy = 0 \quad \Rightarrow \quad c\lambda x + d\mu y = 0 \;\Rightarrow\; \lambda(cx + dy) + (\mu - \lambda)dy = 0 \quad \Rightarrow \quad (\mu - \lambda)dy = 0 \tag{72}$$

But $\mu \neq \lambda$ and $d \neq 0$, so $y = 0$, which contradicts the fact that y is a non-zero vector. So we conclude that eigenvectors corresponding to a pair of distinct eigenvalues are always linearly independent.

• This can be extended to any number of distinct eigenvalues: **Eigenvectors corresponding to a set of distinct eigenvalues are linearly independent**. One can prove this inductively.

• It follows that if an $n \times n$ matrix **has n distinct eigenvalues**, then the corresponding n **eigenvectors are linearly independent and span the whole vector space**. So matrices with n distinct eigenvalues are not deficient.

• **When eigenvalues coincide, their corresponding eigenvectors may remain independent or become collinear. Deficiencies arise in the latter case**.

7.1 More examples of eigenvalues and eigenvectors

• The zero matrix $0_{n\times n}$ annihilates all vectors $0x = x$, so every non-zero vector is an eigenvector with eigenvalue 0. The characteristic equation is $\lambda^n = 0$, so 0 is an eigenvalue with multiplicity n.

• Consider the diagonal matrix $D = \text{diag}(\lambda_1, \lambda_2, \cdots, \lambda_n)$. Let us take $n = 3$ for definiteness. The eigenvalue equation becomes

$$\begin{pmatrix} \lambda_1 x_1 \\ \lambda_2 x_2 \\ \lambda_3 x_3 \end{pmatrix} = \lambda \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix}. \tag{73}$$

The solutions are $\lambda = \lambda_1$ with $x_2 = x_3 = 0$ and x_1 arbitrary (in particular we could take $x_1 = 1$ to get an eigenvector of length 1) and similarly two more. So the eigenvectors can be taken as $\begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$ with eigenvalue λ_1, $\begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}$ with eigenvalue λ_2 and finally $\begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$ with eigenvalue λ_3. Notice that the normalized eigenvectors are just the columns of the identity matrix. The characteristic equation is $(\lambda - \lambda_1)(\lambda - \lambda_2)(\lambda - \lambda_3) = 0$. So the eigenvalues of a diagonal matrix are just its diagonal entries, and the eigenvectors are the corresponding columns of the identity matrix. The determinant is just the product of the diagonal elements.

• The eigenvalues are not always real, consider the rotation matrix

$$A = \begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix}, \det(A - \lambda I) = \det \begin{pmatrix} \cos\theta - \lambda & \sin\theta \\ -\sin\theta & \cos\theta - \lambda \end{pmatrix} = \lambda^2 - 2\lambda\cos\theta + 1 = 0 \tag{74}$$

The roots of the characteristic polynomial are $\lambda = \cos\theta \pm i \sin\theta = e^{\pm i\theta}$, which are generally complex, but lie on the unit circle.

• The **set of eigenvalues is called the spectrum of the matrix**. It is a subset of the complex plane.

• Consider the projection from R^3 to the sub-space spanned by the vector $a = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$, i.e. to the x-axis. $P_a = aa^t = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$. Geometrically, $Px = x$ for precisely those vectors along the x-axis. So a is itself a normalized eigenvector with eigenvalue 1. The 1-eigenspace of P is one-dimensional. Only vectors v orthogonal to the x-axis are annihilated $Pv = 0$. So non-zero vectors in the y-z plane are the eigenvectors with eigenvalue 0. So the 0-eigenspace of A consists of all vectors orthogonal to a. Of course, P_a is a diagonal matrix, so we could have read off its eigenvalues: $\{1, 0, 0\}$.

• The characteristic equation for P_A is $\det(P - \lambda I) = 0$, or $\lambda^2(\lambda - 1) = \lambda(\lambda^2 - \lambda) = 0$. Recall that for a projection matrix, $P^2 = P$. So we make the curious observation that P **satisfies its own characteristic equation** $P(P^2 - P) = 0$.

7.2 Cayley Hamilton Theorem

• One of the most remarkable facts about matrices is that **every matrix satisfies its own characteristic equation**. This is the Cayley-Hamilton theorem.

• Let us first check this in the above example $A = \begin{pmatrix} 1 & 2 \\ 2 & 4 \end{pmatrix}$. The characteristic equation is $\lambda^2 - 5\lambda = 0$. The Cayley-Hamilton theorem says that $A^2 - 5A = 0$. It is easy to check that $A^2 = \begin{pmatrix} 5 & 10 \\ 10 & 20 \end{pmatrix} = 5A$.

• Any matrix $A_{n \times n}$ satisfies its own characteristic equation

$$(A - \lambda_1)(A - \lambda_2) \cdots (A - \lambda_n) \equiv 0 \tag{75}$$

• **Proof of the Cayley-Hamilton theorem.** We will indicate the proof only for non-deficient matrices, i.e., those whose eigenvectors span the whole n-dimensional space. This is the case for matrices with n distinct eigenvalues.

• Essentially, we will show that **every vector is annihilated by the matrix given by the characteristic polynomial** $P(A) = (A - \lambda_1)(A - \lambda_2) \cdots (A - \lambda_n)$. It will follow that $P(A)$ is the zero matrix. Now $(A - \lambda_1)$ annihilates the first eigenvector x_1, $(A - \lambda_1)x_1 = 0$. Now consider $(A - \lambda_2)(A - \lambda_1)$, this matrix annihilates any linear combination of the eigenvectors x_1 and x_2 since the first factor annihilates x_2 and the second annihilates x_1 (the various factors commute). Continuing this way

$$P(A)(a_1 x_1 + a_2 x_2 + \cdots + a_n n_n) = 0 \tag{76}$$

But for a non-deficient matrix, the eigenvectors span the whole space, so $P(A)$ annihilates every vector and must be the zero matrix.

• The Cayley-Hamilton theorem states that a matrix satisfies an n^{th} order polynomial equation

$$A^n + c_{n-1}A^{n-1} + c_{n-2}A^{n-2} + \cdots + c_1 A + c_0 = 0 \tag{77}$$

In other words, we can express A^n in terms of lower powers of A. Similarly any power A^k with $k \geq n$, can be reduced to a linear combination of $I, A, A^2, \cdots, A^{n-1}$

• Returning to the **example** $A = \begin{pmatrix} 1 & 2 \\ 2 & 4 \end{pmatrix}$, let us use the Cayley-Hamilton theorem to calculate A^{20}. Here the characteristic equation satisfied by A reads $A^2 = 5A$. This implies $A^3 = 5A^2 = 5^2 A$, $A^4 = 5^2 A^2 = 5^3 A$, $A^n = 5^{n-1} A$ for $n \geq 2$. Thus we have without having multiplied 20 matrices,

$$A^{20} = 5^{19} A = 5^{19} \begin{pmatrix} 1 & 2 \\ 2 & 4 \end{pmatrix}. \tag{78}$$

7.3 Diagonalization of matrices with n distinct eigenvalues

• **If $A_{n\times n}$ is not deficient (as when it has n distinct eigenvalues), by a suitable invertible change of basis, we can bring it to diagonal form Λ with the diagonal entries of Λ given by the eigenvalues.**

$$A = S\Lambda S^{-1} \quad \text{or} \quad S^{-1}AS = \Lambda. \tag{79}$$

This process is called the **diagonalization** of the matrix. The **invertible change of basis** is called a **general linear** or **similarity transformation** S. If A is **symmetric or hermitian**, it turns out that the **change of basis can be chosen** to be an **orthogonal or unitary** transformation.

• It is important to emphasize that the resulting diagonal matrix of eigenvalues Λ is in general different from the diagonal matrix D that might be obtainable through row elimination in the case when A has n (non-zero) pivots. The pivots are in general different from the eigenvalues. Row elimination involves left multiplication of A by elementary matrices while diagonalization involves left and right multiplication of A by S^{-1} and S.

• We can collect the n eigenvalues of A in the diagonal matrix

$$\Lambda = \begin{pmatrix} \lambda_1 & 0 & \cdots & 0 \\ 0 & \lambda_2 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \cdots & \lambda_n \end{pmatrix}. \tag{80}$$

• And collect the corresponding n eigenvectors x_i satisfying $Ax_i = \lambda_i x_i$ as the columns of a matrix S

$$S = \begin{pmatrix} | & | & \cdots & | \\ x_1 & x_2 & \cdots & x_n \\ | & | & \cdots & | \end{pmatrix}. \tag{81}$$

Then notice that multiplying by columns

$$AS = \begin{pmatrix} Ax_1 & Ax_2 & \cdots & Ax_n \end{pmatrix}, \quad \text{and} \quad S\Lambda = \begin{pmatrix} \lambda_1 x_1 & \lambda_2 x_2 & \cdots & \lambda_n x_n \end{pmatrix}. \tag{82}$$

Then the n solutions of the eigenvalue problem may be summarized as

$$AS = S\Lambda. \tag{83}$$

Similarly we can consider the left eigenvalue problem for A, $y^t A = \mu y^t$ with row eigenvectors y^t. But taking the transpose, this is just the eigenvalue problem for the transpose $A^t y = \mu y$.

• But we know that the eigenvalues of A^t are the same as those of A, so we can write $A^t y_i = \lambda_i y_i$ for the n eigenvectors of A^t. The eigenvectors of A and A^t are in general different, but we will see that they are related. Let us collect the eigenvectors of A^t as the columns of a matrix $T = \begin{pmatrix} y_1 & y_2 & \cdots & y_n \end{pmatrix}$. Then

$$A^t\, T = T\Lambda \qquad \text{and} \qquad AS = S\Lambda. \tag{84}$$

Taking the transpose of these, we can calculate $T^t AS$ in two different ways to get

$$T^t AS = \Lambda T^t S \qquad \text{and} \qquad T^t AS = T^t S\Lambda. \tag{85}$$

Now let $W = T^t S$, then combining, we conclude that W commutes with Λ

$$\Lambda W = W\Lambda \tag{86}$$

In other words,

$$\begin{pmatrix} 0 & (\lambda_1 - \lambda_2)w_{12} & \cdots & (\lambda_1 - \lambda_n)w_{1n} \\ (\lambda_2 - \lambda_1)w_{21} & 0 & \cdots & (\lambda_2 - \lambda_n)w_{2n} \\ \vdots & \vdots & \vdots & \vdots \\ (\lambda_n - \lambda_1)w_{n1} & (\lambda_n - \lambda_2)w_{n2} & \cdots & 0 \end{pmatrix} = 0 \tag{87}$$

Now since the λ's are distinct, we must have $w_{ij} = 0$ for $i \neq j$. Thus $W = T^t S$ is the diagonal matrix

$$W = \begin{pmatrix} w_{11} & 0 & \cdots & 0 \\ 0 & w_{22} & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \cdots & w_{nn} \end{pmatrix} \tag{88}$$

But $W = T^t S$ is merely the matrix of dot products of the eigenvectors of A^t and A, $w_{ij} = y_i^t x_j$. So we have shown that the **left and right eigenvectors of A corresponding to distinct eigenvalues are orthogonal!** We say that the x_i and y_j are in a biorthogonal relation to eachother.

• But the normalization of the eigenvectors was arbitrary. By rescaling the $x_i \mapsto \frac{x_i}{w_{ii}}$ we can make W the identity matrix.

$$W = T^t S = I, \quad y_i^t x_j = \delta_{ij} \tag{89}$$

Now we showed earlier that if A has distinct eigenvalues, its eigenvectors form a linearly independent set. So the columns of S are linearly independent and it is invertible. The same holds for T. So with this normalization, we find that $T^t = S^{-1}$. Putting this in the formula for $T^t AS =$ we get

$$S^{-1}AS = \Lambda \quad \text{or} \quad A = S\Lambda S^{-1} \tag{90}$$

In other words, A may be diagonalized by the general linear transformation (similarity transformation) given by the invertible matrix S whose **columns are** the (appropriately normalized) **eigenvectors** of A!

• Now suppose $A^t = A$ is a symmetric matrix. Then there is no difference between left and right eigenvectors and $S = T$. But since $T^t S = I$, we must have $S^t S = I$ i.e., S is an orthogonal matrix. In other words, a symmetric matrix may be diagonalized by an orthogonal transformation. But the columns of an orthogonal matrix are orthonormal, so we conclude that the **eigenvectors of a symmetric matrix may be chosen orthonormal**. (Actually we have only proved this if the eigenvalues are distinct, though the result is true even if the symmetric matrix has repeated eigenvalues)

• Similarly, a hermitian matrix H may be diagonalized by a unitary transformation U whose columns are the eigenvectors of H. Moreover the eigenvectors are orthogonal and may be taken orthonormal by rescaling them

$$H = U\Lambda U^\dagger, \quad \text{with} \qquad U^\dagger U = I \tag{91}$$

• More generally, a **normal matrix** is one that **commutes with its adjoint**, $A^\dagger A = AA^\dagger$ or $[A^\dagger, A] = 0$. Essentially the same proof as above can be used to show these two statements: If the eigenvectors of a matrix A with distinct eigenvalues are orthogonal, then A is a normal matrix. Conversely, the eigenvectors of a normal matrix with distinct eigenvalues may be taken orthonormal. In fact, more is true A **may be diagonalized by a unitary transformation iff** A **is normal.** Examples of normal matrices include but are not restricted to (anti)-symmetric, orthogonal, (anti)-hermitian and unitary matrices.

• A matrix A is **diagonalizable** if there is a basis where it is diagonal. In other words, it may be **diagonalized by some similarity transformation** S, i.e. $S^{-1}AS = \Lambda$, where Λ is the diagonal matrix with eigenvalues for the diagonal entries. The columns of S are then n linearly independent eigenvectors.

• If a matrix is diagonalizable, the **basis in which it is diagonal is called the eigen-basis**. The eigenbasis consists of n linearly independent eigenvectors. We have shown above that every matrix with n distinct eigenvalues is diagonalizable.

• **Every hermitian or symmetric matrix is diagonalizable.** For example $\sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$ is diagonalizable. Find its eigenvalues and eigenvectors and the unitary transformation that diagonalizes it.

• **Deficient matrices are not diagonalizable.** Proof: Suppose a deficient matrix N were diagonalizable, $S^{-1}NS = \Lambda$. Then the columns of S would be n linearly independent eigenvectors of N. But a deficient matrix does not possess n linearly independent eigenvectors! Contradiction.

• Eg: The matrix $N = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$ is not diagonalizable. 0 is an eigenvalue with algebraic multiplicity 2 but geometric multiplicity one. N has only one eigenvector.

• **Simultaneous diagonalizability:** A pair of matrices $A, B : V \to V$ are said to be simultaneously diagonalizable if the **same similarity transformation** S **diagonalizes them both** i.e. $S^{-1}AS = \Lambda_A$ and $S^{-1}BS = \Lambda_B$. Here Λ_A and Λ_B are the diagonal matrices with eigenvalues of A and B along the diagonal respectively. Now the invertible matrix S contains the eigenvectors of A and B, so A and B **share the same eigenvectors** (though they may have different eigenvalues). Since S is invertible, the eigenvectors span the whole vector space V.

• If A and B are **simultaneously diagonalizable, then they commute**. $S^{-1}AS = \Lambda_A$ and $S^{-1}BS = \Lambda_B$. Now $[\Lambda_A, \Lambda_B] = 0$ as can be checked using the fact that they are diagonal. By the invariance of matrix equations under similarity transformations we conclude that $[A, B] = 0$. **If they commute in one basis, they commute in any other basis.**

• Sufficient criterion for simultaneous diagonalizability. Suppose A has n distinct eigenvalues and that a matrix B commutes with A, $[A, B] = 0$. Then B and A are simultaneously diagonalizable.

• Proof: Suppose x is an eigenvector of A with eigenvalue λ, $Ax = \lambda x$. Then we will show that x is also an eigenvector of B. Consider λBx, which can be written as $\lambda Bx = BAx = ABx$. So $A(Bx) = \lambda(Bx)$. x was already an eigenvector of A with eigenvalue λ. Now we found that Bx is also an eigenvector of A with eigenvalue λ. Since A has distinct eigenvalues, its eigenspaces are one dimensional and therefore Bx must be a multiple of x, i.e., $Bx = \mu x$. So we have shown that any eigenvector of A is also an eigenvector of B. Since the eigenvectors of A span the whole vector space we conclude that A and B have common eigenvectors and are simultaneously diagonalizable.

• Remark: We can replace the assumption that A have n distinct eigenvalues with some other hypotheses. For example we could assume that A and B both be hermitian and commuting. Then it is still true that they are simultaneously diagonalizable.

• Eg: **Pauli matrices do not commute and they are not simultaneously diagonalizable.** For example $[\sigma_2, \sigma_3] = i\sigma_1$ with $\sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$. Check that the unitary transformation that makes σ_2 diagonal forces σ_3 to become non-diagonal.

• Suppose A is invertible (in particular 0 is not an eigenvalue of A). Then eigenvalues of A^{-1} are the **reciprocals of the eigenvalues** of A. This is why:

$$Ax = \lambda x \quad \Rightarrow \quad A^{-1}Ax = \lambda A^{-1}x \quad \Rightarrow \quad A^{-1}x = \frac{1}{\lambda}x \tag{92}$$

In fact, this shows that the eigenvector corresponding to the eigenvalue $\frac{1}{\lambda}$ of A^{-1} is the same as the eigenvector x of A corresponding to the eigenvalue λ. They have the same corresponding eigenvectors. In particular, if A was diagonalizable, then A^{-1} is diagonalizable simultaneously.

• Caution: **An invertible matrix may not be diagonalizable.** For example $N = \begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix}$ is invertible but not diagonalizable. It has only one linearly independent eigenvector, $\begin{pmatrix} 1 \\ 0 \end{pmatrix}$ corresponding to the twice repeated eigenvalue $\lambda = 1$. $\lambda = 1$ has algebraic multiplicity two but geometric multiplicity only one. N is deficient. There is no basis in which N is diagonal.

7.4 Quadratic surfaces and principle axis transformation

• There is a **geometric interpretation** of the **diagonalization of a symmetric matrix**. It is called the **principal axis transformation**.

• In analytic geometry, the equation for an **ellipse** on the plane is usually given as

$$\frac{x^2}{a^2} + \frac{y^2}{b^2} = 1 \tag{93}$$

In this form, the major and minor axes are along the cartesian coordinate axes. Similarly, the equation of an **ellipsoid** embedded in 3d Euclidean space is often given as

$$\frac{x^2}{a^2} + \frac{y^2}{b^2} + \frac{z^2}{c^2} = 1 \tag{94}$$

Since it is defined by a quadratic equation, the ellipsoid is called a **quadratic surface**. The lhs involves terms that are purely quadratic in the variables. Such an expression (lhs) is called a **quadratic form**.

• More generally, an ellipsoid in n-D space with axes along the cartesian coordinate axes is

$$\lambda_1 x_1^2 + \lambda_2 x_2^2 + \cdots + \lambda_n x_n^2 = 1 \tag{95}$$

This can be regarded as a matrix equation $x^t \Lambda x = I$ for the column vector $x = (x_1, x_2, \cdots, x_n)^t$ and diagonal matrix $\Lambda = \text{diag}(\lambda_1, \lambda_2, \cdots, \lambda_n)$. $x^t \Lambda x$ is called the **quadratic form associated to** Λ.

• However, often we are confronted with quadratic surfaces that are not aligned with the coordinate axes, but are in an arbitrarily rotated position. The equation for such a surface is again quadratic but with cross-terms of the form $x_i x_j$. For example

$$ax^2 + by^2 + cxy + dyx = 1 \tag{96}$$

But since $xy = yx$, only $c+d$ contributes, so we could have taken the coefficients of xy and yx to both equal $\frac{c+d}{2}$. More generally we have a quadratic equation

$$x_i A_{ij} x_j = 1 \quad \text{or} \quad x^t A x = 1 \tag{97}$$

where we may assume that $A_{ij} = A_{ji}$ is a **real symmetric matrix**.

• At each point P on the surface we have a **normal direction** to the surface, one that is normal (perpendicular) **to the tangential plane** to the surface through P.

• There is also the **radius vector** ('position vector' from the origin) x of the point P. In general, the position vector and normal do not point along the same direction.

• The **principal axes** are defined as those **radius vectors which point along the normal**.

• In general, the **normal to the surface at x points along Ax**. To see this we first observe that if x lies on the surface, then a neighboring vector $x + \delta x$ also lies approximately on the surface if $(x+\delta x)^t A (x+\delta x) = 1$ up to terms quadratic in δx. In other words, $x^t A \delta x + \delta x^t A x = 0$, or $\delta x^t A x = 0$ as A is symmetric. Such δx are the tangent vectors to the surface at x. But this is just the statement that δx must be normal to Ax. So the normal vector must be along Ax.

• So the condition for x to be a **principal axis** is that it must be **proportional to the normal** Ax, or $Ax = \lambda x$, which is just the **eigenvalue equation**.

• Moreover, the **eigenvalue has a geometric interpretation**. Suppose x is a principal axis of A through P. Then $x^t A x = \lambda x^t x = 1$ So $x^t x = \frac{1}{\lambda}$. But $x^t x$ is the square of the length of the position vector. So $\frac{1}{\lambda}$ is the **square of the length of the semi-axis** through P.

• Since A is symmetric, from the last section, we know that its eigenvectors are orthogonal. In other words, the principal axes are orthogonal. However, the principal axes may not point along the original cartesian coordinate axes. But if we take our new coordinate axes to point along the principal axes, then A is diagonal in this new basis. More precisely, A is diagonalized by an orthogonal transformation

$$Q^t A Q = \Lambda \tag{98}$$

where the columns of Q are the eigenvectors, $Q^t Q = I$ and Λ is the diagonal matrix of eigenvalues. So if we let $y = Q^t x$ then the equation of the surface $x^t A x = 1$ becomes $x^t Q \Lambda Q^t x = 1$ or simply $y^t \Lambda y$.

• In this geometric interpretation, we have implicitly assumed that the eigenvalues are real and that the eigenvectors are real vectors (for a real symmetric matrix). This is indeed true, as we will show in the next section.

• Finally, we point out the geometric meaning of coincidence of eigenvalues. Suppose $n = 2$, and suppose we have transformed to the principal axes. Then we have an ellipse $\lambda_1 x^2 + \lambda_2 y^2 = 1$ whose principal axes are along the x and y axes. Now if the eigenvalues gradually approach each other, $\lambda_1, \lambda_2 \to \lambda$ the ellipse turns into a circle. At the same time the diagonal matrix $\Lambda = \begin{pmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{pmatrix}$ tends to the multiple of the identity $\Lambda \to \begin{pmatrix} \lambda & 0 \\ 0 & \lambda \end{pmatrix}$. But every vector is an eigenvector of λI. In particular, we are free to pick any pair of orthogonal vectors and call them the principal axes of the circle.

• So when **eigenvalues of a symmetric matrix coincide**, the matrix **does not become deficient** in eigenvectors. It still possesses a system of n orthogonal eigenvectors, but some of them are no longer uniquely determined.

7.5 Spectrum of symmetric or hermitian matrices

• A real symmetric matrix is a real matrix $A : R^n \to R^n$ which equals its transpose $A = A^t$. A hermitian matrix is a complex matrix $H : C^n \to C^n$ whose transpose is its complex conjugate: $(H^t)^* = H$, also written as $H^\dagger = H$. A special case is a real symmetric matrix. So every real symmetric matrix is also hermitian. Examples: The Pauli matrix $\sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$ is hermitian but not symmetric. The Pauli matrix $\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$ is hermitian and symmetric.

• **The diagonal matrix elements of H in any basis are real.** In other words, let $z \in C^n$ be any vector, then $(z, Hz) = z^\dagger H z \in R$. To see this, take the complex conjugate of $z^t H z$, which is the same as the hermitian adjoint of the 1×1 matrix $z^\dagger H z$,

$$(z^\dagger H z)^* = (z^\dagger H z)^\dagger = z^\dagger H^\dagger z = z^\dagger H z. \tag{99}$$

So $z^\dagger H z$ is a number that equals its own complex conjugate, it must be real! In quantum mechanics (QM), $(z, Hz)/(z, z)$ is called the **normalized expectation value** of H in the state z.

• Eg: The 3D representation of angular momentum matrices in QM are these hermitian matrices

$$L_x = \frac{1}{2}\begin{pmatrix} 0 & \sqrt{2} & 0 \\ \sqrt{2} & 0 & \sqrt{2} \\ 0 & \sqrt{2} & 0 \end{pmatrix}; \quad L_y = \frac{1}{2i}\begin{pmatrix} 0 & \sqrt{2} & 0 \\ -\sqrt{2} & 0 & \sqrt{2} \\ 0 & -\sqrt{2} & 0 \end{pmatrix}; \quad L_z = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix} \tag{100}$$

• **The eigenvalues of a hermitian matrix are real.** Suppose z is an eigenvector with eigenvalue λ, i.e., $Hz = \lambda z$. Taking the inner product with z,

$$(z, Hz) = z^\dagger H z = z^\dagger \lambda z = \lambda ||z||^2 \Rightarrow \lambda = \frac{(z, Hz)}{||z||^2} \tag{101}$$

$z^\dagger z = |z_1|^2 + \cdots |z_n|^2$ is real. Being the ratio of two real quantities, the eigenvalue λ is real.

• Example: Check that the eigenvalues of σ_2 are real.

• **Eigenvectors of a hermitian matrix corresponding to distinct eigenvalues are orthogonal.** Proof: Suppose z, w are two eigenvectors, $Hz = \lambda z$ and $Hw = \mu w$, with eigenvalues $\lambda \neq \mu$, which are necessarily real. Then $w^\dagger H z = \lambda w^\dagger z$ and $z^\dagger H w = \mu z^\dagger w$. But the lhs are complex conjugates of each other, $(w^\dagger H z)^* = (w^\dagger H z)^\dagger = z^\dagger H w$. So $\lambda w^\dagger z = (\mu z^\dagger w)^*$. Or we have $w^\dagger z(\lambda - \mu) = 0$. By distinctness, $\lambda \neq \mu$, so $w^\dagger z = 0$ and w, z are orthogonal.

• Find the eigenvectors of σ_2 and show they are orthogonal.

• More generally, even if H has a repeated eigenvalue, we can still choose an orthogonal basis for the degenerate eigenspace so that eigenvectors of a hermitian matrix can be chosen orthogonal.

• **Eigenvectors of a real symmetric matrix may be chosen real.** This is important for the geometric interpretation of the eigenvectors as principal axes of an ellipsoid. We will assume that the eigenvalues are distinct. **Proof:** We are given a real ($A^* = A$) symmetric matrix, so its eigenvalues are real. Suppose z is a possibly complex eigenvector corresponding to the eigenvalue $\lambda = \lambda^*$, i.e., $Az = \lambda z$. Taking the complex conjugate, $A^* z^* = \lambda^* z^*$ or $Az^* = \lambda z^*$, so z^* is also an eigenvector with the same eigenvalue. So $x = z + z^*$ is a real eigenvector with eigenvalue λ. So for every eigenvalue we have a real eigenvector. [The eigenspaces of A are 1-dimensional since we have n distinct eigenvalues and the corresponding eigenvectors must be orthogonal. So z and z^* are (possibly complex) scalar multiples of x.]

• Exercise: Check that if H is hermitian, iH is anti-hermitian.

7.6 Spectrum of orthogonal and unitary matrices

• Orthogonal matrices are those real matrices that satisfy $Q^t Q = Q Q^t = I$. The columns (and rows) of an orthogonal matrix are orthonormal. Unitary matrices are complex matrices satisfying $U^\dagger U = 1$. If a unitary matrix happens to be real, then it is necessarily orthogonal. The columns (and rows) of a unitary matrix are orthonormal.

• A rather simple example of an orthogonal matrix is a *reflection* in the x axis, $Q = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$. This happens to be diagonal. so the eigenvalues are $+1$ and -1, and the corresponding eigenvectors are the columns of the 2×2 identity matrix. Another example of an orthogonal matrix is the *rotation* matrix

$$A = \begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix}, \det(A - \lambda I) = \det \begin{pmatrix} \cos\theta - \lambda & \sin\theta \\ -\sin\theta & \cos\theta - \lambda \end{pmatrix} = \lambda^2 - 2\lambda\cos\theta + 1 = 0 \tag{102}$$

The roots of the characteristic polynomial are $\lambda = \cos\theta \pm i \sin\theta = e^{\pm i\theta}$, which are generally complex, but lie on the unit circle.

• **Eigenvalues of orthogonal and unitary matrices lie on the unit circle in the complex plane.** This follows from the fact that orthogonal $Q^t Q = I$ and unitary $U^\dagger U = I$ matrices are isometries. They preserve the lengths of vectors: $||Qx|| = ||x||$ and $||Ux|| = ||x||$. So if we consider an eigenvector $Qv = \lambda v$, we have $||\lambda v|| = ||v||$ or $|\lambda|\ ||v|| = ||v||$, which implies $|\lambda| = 1$. The same works for unitary matrices.

• To see that orthogonal transformations are isometries, consider $||Qx||^2 = (Qx)^t Qx = x^t Q^t Qx = x^t x = ||x||^2$ since $Q^t Q = I$. Taking the positive square root, $||Qx|| = ||x||$ for all vectors x.

• **Eigenvectors of unitary matrices corresponding to distinct eigenvalues are orthogonal**.

• Proof: Suppose z, w are eigenvectors corresponding to distinct eigenvalues $\lambda \neq \mu$, $Uz = \lambda z$ and $Uw = \mu w$. Then we want to show that $z^\dagger w = 0$. So take the adjoint of the first equation $z^\dagger U^\dagger = \lambda^* z^\dagger$ and multiply it with the second and use $U^\dagger U = I$

$$z^\dagger U^\dagger U w = \lambda^* \mu z^\dagger w \quad \text{or} \quad (1 - \lambda^* \mu) z^\dagger w = 0 \tag{103}$$

But since $\lambda^* \lambda = 1$ and $\lambda \neq \mu$ we have that $\lambda^* \mu \neq 1$. So the second factor must vanish, $z^\dagger w = 0$ and z and w are orthogonal.

• Remark: **If H is hermitian, $U = e^{iH}$ is unitary**.

7.7 Exponential and powers of a matrix through diagonalization

• **Powers of a matrix are easily calculated once it is diagonalized**. If $A = S\Lambda S^{-1}$, and $n = 0, 1, 2, \ldots$

$$A^n = (S\Lambda S^{-1})^n = S\Lambda^n S^{-1} \tag{104}$$

Moreover, Λ^n is just the diagonal matrix with the n^{th} powers of the eigenvalues along its diagonal entries.

• Exponential of a matrix through diagonalization. If a matrix can be diagonalized by a similarity transformation $A = S\Lambda S^{-1}$, then calculating its exponential e^A is much simplified

$$e^A = e^{S\Lambda S^{-1}} = \sum_{n=0}^{\infty} \frac{(S\Lambda S^{-1})^n}{n!} = \sum_n \frac{S\Lambda^n S^{-1}}{n!} = S e^\Lambda S^{-1} \tag{105}$$

So we just apply the similarity transformation to e^Λ to get e^A. Moreover, since Λ is a diagonal matrix, its exponential is easy to calculate. If $\Lambda = diag(\lambda_1, \cdots, \lambda_n)$, then

$$e^\Lambda = diag(e^{\lambda_1}, e^{\lambda_2}, e^{\lambda_3}, \cdots, e^{\lambda_n}) \tag{106}$$

7.8 Coupled oscillations via diagonalization

• **Small displacements** of a system about a point of **stable equilibrium** typically lead to **small oscillations** due to **restoring forces**. They are described by linearizing the equations of motion, assuming the departure from equilibrium is small. Hookes law for a slightly elongated spring is an example. If δx is the small displacement, Newton's law in Hooke's approximation says $m\ddot{\delta x} = -k\ \delta x$. This is a linear equation for one unknown function $\delta x(t)$.

• Similarly, suppose we have a pair of equally massive objects in one dimension connected by a spring to each other and also by springs to walls on either side in this order: **wall spring mass**

spring mass spring wall. Let $\delta x_1, \delta x_2$ be **small displacements** of the masses to the right. Draw a diagram of this configuration. Newton's equations in Hooke's approximation (when the springs have the same spring constant k) are

$$\begin{aligned} m\delta \ddot{x}_1 &= -k\delta x_1 + k(\delta x_2 - \delta x_1) \\ m\delta \ddot{x}_2 &= -k\delta x_2 - k(\delta x_2 - \delta x_1) \end{aligned} \tag{107}$$

This is a pair of **coupled differential equations**; it is not easy to solve them as presented. But we can write them as a single **matrix differential equation** $\ddot{x} = Ax$ were $x = \begin{pmatrix} \delta x_1 \\ \delta x_2 \end{pmatrix}$

$$\frac{d^2}{dt^2}\begin{pmatrix} \delta x_1 \\ \delta x_2 \end{pmatrix} = \frac{k}{m}\begin{pmatrix} -2 & 1 \\ 1 & -2 \end{pmatrix}\begin{pmatrix} \delta x_1 \\ \delta x_2 \end{pmatrix}. \tag{108}$$

Let $A = \frac{k}{m}\begin{pmatrix} -2 & 1 \\ 1 & -2 \end{pmatrix}$. **The off-diagonal terms** in A are responsible for the **coupled nature** of the equations. But A is **real symmetric**, so it can be **diagonalized**, which will make the equations **uncoupled**. Upon performing the principal axis transformation, $A = Q\Lambda Q^t$ where $\Lambda = \frac{k}{m}\begin{pmatrix} -1 & 0 \\ 0 & -3 \end{pmatrix}$ is the diagonal matrix of eigenvalues and Q is the orthogonal eigenvector matrix (which is independent of time, since A is). The equations become

$$\ddot{x} = Q\Lambda Q^t x \;\Rightarrow\; Q^t\ddot{x} = \Lambda Q^t x \tag{109}$$

So let $y = Q^t x$, then we get $\ddot{y} = \Lambda y$ which are the pair of uncoupled equations

$$\ddot{y}_1 = -(k/m)y_1, \qquad \ddot{y}_2 = -3(k/m)y_2 \tag{110}$$

If the initial condition was that the masses started from rest, then $\dot{y}(0) = 0$ and the solutions are

$$y_1(t) = y_1(0)\cos(\sqrt{\frac{k}{m}}t) y_2(t) = y_2(0)\cos(\sqrt{\frac{3k}{m}}t) \tag{111}$$

The method of solving these differential equations will be treated in the second part of this course. To get back $x(t)$ we just use $x(t) = Qy(t)$. So it only remains to find the eigenvector matrix Q, of A, which is left as an exercise.

8 Volume element: Change of integration variable and Jacobian determinant

• An important application of determinants is in the change of volume element when (non-linearly) changing integration variables in multi-dimensional integrals.

• An invertible square matrix A can be regarded as a linear change of variable from the standard o.n. basis $(x_i)_j = \delta_{ij}$ to a new basis $\mathbf{y}_i$ given by the columns of A:

$$I = \begin{pmatrix} | & \cdots & | \\ x_1 & \cdots & x_n \\ | & \cdots & | \end{pmatrix}; A = \begin{pmatrix} | & \cdots & | \\ y_1 & \cdots & y_n \\ | & \cdots & | \end{pmatrix}; \tag{112}$$

$\mathbf{y}_i = A\mathbf{x}_i$ or $(y_i)_j = A_{jk}(x_i)_k = A_{ji}$. (Thus A is the derivative of y with respect to x evaluated at $(x_i)_j = \delta_{ij}$: $A_{jk} = \frac{\partial (y_i)_j}{\partial (x_i)_k}$). Under this change of variable, the unit hypercube (whose edges are $\mathbf{x}_i$) is transformed into a parallelepiped whose edges are the columns $\mathbf{y}_i$ of A. So the volume of the parallelepiped formed by the basis vectors is multiplied by $\det A$.

• Now we would like to apply this idea to differentiable non-linear changes of variable. This is given by a function from $R^n \to R^n$: $(x_1 \cdots x_n) \mapsto (y_1(\mathbf{x}), \cdots y_n(\mathbf{x}))$. A non-linear change of variable can be approximated by an affine (linear + shift) one in a small neighbourhood of any point x', $y_i(x) = y_i(x') + J_{ij}(x-x')_j + \cdots$. Up to an additive constant shift, this linear transformation is the *linearization* of y, or the Jacobian matrix $J_{ij} = \frac{\partial y_i}{\partial x_j}$ where the derivatives are evaluated at $x = x'$. So near each point, the unit hyper cube is transformed to a parallelepiped whose volume is $\det J$. The Jacobian matrix is $J_{ij}(\mathbf{x}) = \frac{\partial y_i}{\partial x_j}$ and the Jacobian determinant is $\det J_{ij}$.

• The change of variable formula for volume elements is

$$|\det J| \; dx_1 \cdots dx_n = dy_1 \cdots dy_n \tag{113}$$

So that

$$\int dy_1 \cdots dy_n \; f(\mathbf{y}) \;=\; \int dx_1 \cdots dx_n \;\; |\det J(\mathbf{x})| \;\; f(\mathbf{y}(\mathbf{x})) \tag{114}$$

For transformation from cartesian to plane polar coordinates $x = r\cos\theta, y = r\sin\theta$

$$dx\; dy \;=\; dr\; d\theta\; \det\begin{pmatrix} \frac{\partial x}{\partial r} & \frac{\partial x}{\partial \theta} \\ \frac{\partial y}{\partial r} & \frac{\partial y}{\partial \theta} \end{pmatrix} = dr\; d\theta\; \det\begin{pmatrix} \cos\theta & -r\sin\theta \\ \sin\theta & r\cos\theta \end{pmatrix} = r\; dr\; d\theta. \tag{115}$$

• Ex. Work out the Jacobian determinant for transformation from cartesian to spherical polar coordinates. $z = r\cos\theta$, $x = r\sin\theta\cos\phi$, $y = r\sin\theta\sin\phi$.

• Note: The Jacobian matrix of the gradient of a function is the Hessian matrix of second partials.