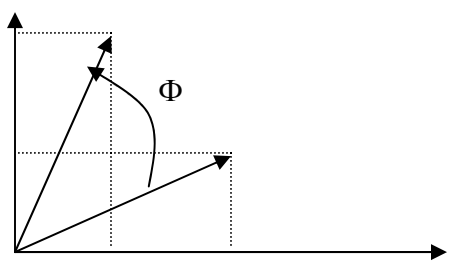
Rotation matrices

We consider now rotation matrices in two and three dimensions. We start with two dimensions since two dimensions are easier than three to understand, and one dimension is a little too simple. However, our prime interest is in three dimensions, where proteins are embedded.

We expect from rotation matrices to have the following properties: U is a square real matrix such that $UU^t = I$ (which means that the rotation matrix does not change the length of the vector. See below) and $\det(U) = 1$ (which means that we do not allow mirror images).

Let us start with a two dimensional case. We consider a vector (x, y) that we wish to rotate in the plane by an angle Φ (in the direction opposite to the clock). The norm of the vector is kept fixed. The diagram below describes the operation of interest



It is possible to think about the rotation of the vector (x, y) as a rotation of two vectors $(x, 0)$ and $(0, y)$ which we will finally add up to a single operation (it is more convenient too!). Consider first the vector component $x \equiv (x, 0)$ and the effect of the rotation on it. Rotating by Φ the vector $(x, 0)$ modifies the old into a new vector $(x\cos(\Phi), x\sin(\Phi))$. Similarly for the y component of the vector $(0, y)$ we find that counter clockwise rotation by an angle Φ generates the vector $(-y\sin(\Phi), y\cos(\Phi))$. The complete new vector after the rotation will be
$(x\cos(\Phi) - y\sin(\Phi), x\sin(\Phi) + y\cos(\Phi))$

The above operation which we did by using geometry and some intuition can be put in a more elegant form using a rotation matrix

$$U(\Phi) = \begin{pmatrix} \cos(\Phi) & -\sin(\Phi) \\ \sin(\Phi) & \cos(\Phi) \end{pmatrix}$$

$$\begin{pmatrix} \cos(\Phi) & -\sin(\Phi) \\ \sin(\Phi) & \cos(\Phi) \end{pmatrix}\begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} x\cos(\Phi) - y\sin(\Phi) \\ x\sin(\Phi) + y\cos(\Phi) \end{pmatrix}$$

Some properties of U

$$UU^t = \begin{pmatrix} \cos(\Phi) & -\sin(\Phi) \\ \sin(\Phi) & \cos(\Phi) \end{pmatrix}\begin{pmatrix} \cos(\Phi) & \sin(\Phi) \\ -\sin(\Phi) & \cos(\Phi) \end{pmatrix} =$$

$$= \begin{pmatrix} \cos^2(\Phi) + \sin^2(\Phi) & \cos(\Phi)\sin(\Phi) - \sin(\Phi)\cos(\Phi) \\ \sin(\Phi)\cos\Phi - \cos(\Phi)\sin(\Phi) & \sin^2(\Phi) + \cos^2(\Phi) \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = I$$

$$\det(U) = \begin{vmatrix} \cos(\Phi) & -\sin(\Phi) \\ \sin(\Phi) & \cos(\Phi) \end{vmatrix} = \cos^2(\Phi) + \sin^2(\Phi) = 1$$

Rotation back by "$-\Phi$" should bring us to the place in which we started (i.e., $U(\Phi)U(-\Phi) = I \quad \rightarrow \quad U(-\Phi) = U^t(\Phi)$. Indeed we have

$$U(-\Phi) = \begin{pmatrix} \cos(-\Phi) & -\sin(-\Phi) \\ \sin(-\Phi) & \cos(-\Phi) \end{pmatrix} = \begin{pmatrix} \cos(\Phi) & \sin(\Phi) \\ -\sin(\Phi) & \cos(\Phi) \end{pmatrix} = U^t(\Phi)$$

Let $\Phi = \phi_1 + \phi_2$, we intuitively expect that the rotation by a sum can be described as sequence of rotations, i.e. $U(\Phi) = U(\phi_1)U(\phi_2)$

A proof:

$$U(\phi_1)U(\phi_2) = \begin{pmatrix} \cos(\phi_1) & -\sin(\phi_1) \\ \sin(\phi_1) & \cos(\phi_1) \end{pmatrix}\begin{pmatrix} \cos(\phi_2) & -\sin(\phi_2) \\ \sin(\phi_2) & \cos(\phi_2) \end{pmatrix} =$$

$$\begin{pmatrix} \cos(\phi_1)\cos(\phi_2) - \sin(\phi_1)\sin(\phi_2) & -\cos(\phi_1)\sin(\phi_2) - \sin(\phi_1)\cos(\phi_2) \\ \sin(\phi_1)\cos(\phi_2) + \cos(\phi_1)\sin(\phi_2) & -\sin(\phi_1)\sin(\phi_2) + \cos(\phi_1)\cos(\phi_2) \end{pmatrix} =$$

$$\begin{pmatrix} \cos(\phi_1 + \phi_2) & -\sin(\phi_1 + \phi_2) \\ \sin(\phi_1 + \phi_2) & \cos(\phi_1 + \phi_2) \end{pmatrix} = \begin{pmatrix} \cos(\Phi) & -\sin(\Phi) \\ \sin(\Phi) & \cos(\Phi) \end{pmatrix} = U(\Phi)$$

Consider a vector V. A rotation matrix U does not change the norm of the vector. Hence $V^tV = (UV)^t(UV)$. This is trivial to show once we remember that $(UV)^t = V^tU^t$, we therefore have

$$(UV)^t \cdot (UV) = V^tU^t(UV) = V^t(U^tU)V = V^tV$$

The distance between any two points is not changing by rotation. Consider two points in the plane: (x_1, y_1) and (x_2, y_2). The distance between the two points, d_{12}, is defined as the norm of the vector difference $d_{12} = \left| \begin{pmatrix} x_1 - x_2 \\ y_1 - y_2 \end{pmatrix} \right| = \sqrt{(x_1 - x_2)^2 + (y_1 - y_2)^2}$ but we just showed that the length of a vector does not change upon rotation. The distance is the length of the vector difference and cannot change by rotation.

We define a "rigid body transformation" as a change in the coordinates that does not affect the distance between any two points of the rigid body (we also require that no mirror imaging takes place).

Note that not all the matrices satisfying $UU^t = I$ are proper rotations. For example for $U = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$ we still have $UU^t = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = I$. However for the second condition mentioned above $(\det(U) = 1)$ we have -- $\det(U) = 1 \cdot (-1) = -1$ which is not a proper rotation.

Another way of thinking about the condition on the determinant above is to consider small rotations. As we have seen a rotation by an angle Φ can be divided to a sequence of small rotations. We can make a large number of such divisions and approach infinitesimal rotations. We write

$$\Phi = \lim_{N \to \infty} \sum_{i=1,..,N} \left(\Phi / N \right)$$

or

$$U(\Phi) = \prod_{i=1,...,N} U(\Phi/N) \qquad U(\Phi/N) \simeq \begin{pmatrix} 1 & -\Phi/N \\ \Phi/N & 1 \end{pmatrix}$$

Such decomposition should always be possible for a real rotation (one has to be careful though when applying such limits. The matrix of an infinitesimal rotation, as written, does not satisfy the condition we set for a rotation). Without proof we comment that matrices with determinant –1 cannot be decomposed to a product of infinitesimal rotation. This can be used as yet another definition of rotation matrices (we must be able to decompose them to a product of smaller rotations).

The matrix we just considered, $\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$ reflects the Y axis through the origin and generates a mirror image. It is impossible to find a sequence of small rotations that takes a vector continuously from the two reflection states of the Y axis.

<u>Rotations in three dimensions</u>

Rotations in three dimensions are a simple extension of the rotations in two dimensions we just discussed. The difference is that in three dimensions we must define a rotation axis. The two dimensional rotations we considered so far can be thought as a special case

of rotations in three dimensions in which the axis of rotation is the Z axis. Consider the following matrix:

$$U = \begin{pmatrix} \cos(\Phi) & -\sin(\Phi) & 0 \\ \sin(\Phi) & \cos(\Phi) & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

when applied onto a vector in three dimensions $v = (x, y, z)$ the result is:

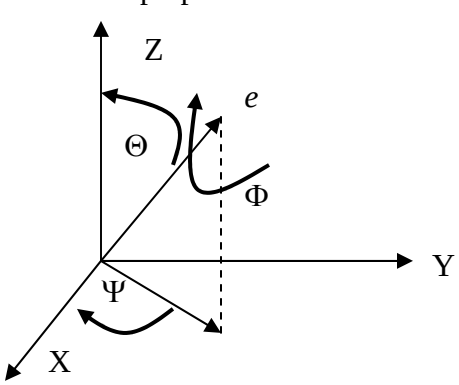
$$Uv = \begin{pmatrix} \cos(\Phi) & -\sin(\Phi) & 0 \\ \sin(\Phi) & \cos(\Phi) & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} x\cos(\Phi) - y\sin(\Phi) \\ x\sin(\Phi) + y\cos(\Phi) \\ z \end{pmatrix}$$

which is exactly the same result we have for a rotation in two dimensions in the xy plane. Here Z is the rotation axis which (in general) remains unchanged when we applied the rotation on a vector along its direction. We can find the rotation axis of an arbitrary rotation matrix in three dimension by solving the following linear problem

$$Ue = 1 \cdot e$$

where e is a vector along the axis of rotation. Since the axis of rotation is not changing when U multiplies it (otherwise it is NOT the axis of rotation), it must be an eigenvector of U with an eigenvalue of 1. Determining e is a linear problem that can be solved (for example) using the Gaussian elimination we discussed earlier. Note that if we multiply e by any scalar we still obtain a valid solution. We therefore choose e to be real (If there is a solution it can be made real since the matrix and the eigenvalue are real) and normalized it to one: $e^t e = 1$. The axis of rotation is therefore determined with only two parameters – two angles (the third is determined by the normalization). The two parameters can be chosen as the relative position of the axis of rotation with respect to the Z axis -- $\cos(\Theta)$ and the angle of the axis of rotation with respect to X axis. The last is obtained by projecting the axis of rotation first to the XY plane and then measuring the relative position with respect to the X axis -- $\cos(\Psi)$.

The sketch below demonstrates the process and the way we define a rotation in three dimensions. As before Φ is a rotation in a plane. The plane is now determined as the set of vectors perpendicular to the axis of rotation. I.e. the set of vectors perpendicular to e



A rotation in three dimensions is therefore completely determined by three parameters: (Θ, Ψ, Φ). Of course the choice of the 3 parameter is unique and there are other ways of uniquely determining a rotation in space, a common example are the Euler angles that can be found in any textbook on classical mechanics (e.g. Goldstein).

As we noted before the determinant of a rotation matrix is 1. What does it say on the range of eigenvalues that a rotation matrix may have?

We spend considerable time on rotation matrices because we have a very concrete question about these matrices. Given two protein structures (modeled as rigid bodies) what kind of rotation we can apply on one of them so that the two structures will overlap as best as possible. Hence we are back to proteins and biology…