Theory of three dimensional reconstruction.'
I. Conditions for a complete set of projections

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Conditions are given under which the set of projections of the three-dimensional function contains complete information about it.

1. INTRODUCTION

The optics of the electron microscope are such that the microphotograph of a biomacromolecule is the projection of its density distribution, as discussed in ref. 1. The problem of recovering the density of the object from the given projections is the basic problem of electron microscopy of biomacromolecules.

In ref. 2 the authors considered the case of coaxial projection when the two projected directions are perpendicular to the fixed axis. The problem of recovering the structure was accomplished, in this case, by using Radon's equation from ref. 3.

The aim of this article is to study the general case, when the projection directions occupy a certain domain on the sphere of directions.

2. POSING THE PROBLEM

Mathematically the problem is formulated as follows. Let $\rho(x)$ be a finite function describing the structure of some object. The projection of this object along the line passing through x and having the direction τ is given by the integral

$$\rho(\mathbf{x}, \tau) = \int_{-\infty}^{\infty} \rho(\mathbf{x} + \tau t)\, dt. \qquad (1)$$

The function $\rho(x, \tau)$ is not a function of the three-dimensional vector x, but of the two-dimensional vector $x - \tau(x\tau)$, perpendicular to the vector τ. It does not depend on the sign of τ, and it describes the structure of the two-dimensional projection of the given object. For brevity, we denote it by (τ).

Suppose we know the projections (τ) along a continuous set of directions[1] $\{\tau\}$. The problem of decoding the structure of the object under consideration is reduced to the solution of the integral equation (1) defined for all x and all $\tau \in \{\tau\}$, i.e., to the finding of a recovery operator $R\{\tau\}$.

$$\rho(\mathbf{x}) = R\{\tau\}\rho(\mathbf{x}, \tau). \qquad (2)$$

3. CONDITIONS FOR THE EXISTENCE OF A SOLUTION

We shall first show that for sets $\{\tau\}$ the problem has a solution. In what follows these sets will be called complete sets. Take the unit sphere of directions S. Each vector $\tau \in \{\tau\}$ is represented on it by a point P_τ, and the set $\{\tau\}$ is a certain closed domain[2] G_τ.

We now show that in order to recover $\rho(x)$ it is necessary and sufficient that G_τ have points in common with any arc of a great circle. To prove this we note that if some projection $\rho(x, \tau)$ is known, then the Fourier transform of the function $\rho(x)$ can be found for all directions lying in the plane orthogonal to the vector τ. Whence it follows, for example, that if a certain arc of a great circle has at least one point in common with G_τ, then the Fourier transform of the function $\rho(x)$ can be found in the direction perpendicular to the plane of this circle. If any arc of a great circle has points in common with G_τ, then the Fourier transform of the function $\rho(x)$ can be found for any direction, and therefore in this case it will be possible to recover $\rho(x)$.

Now let the domain G_τ be such that there is an arc L of the great circle which does not have points in common with G_τ. Since G_τ is closed, each point of this arc L has its own ε-neighborhood in which there are no points of G_τ. This means that the Fourier transform of the function $\rho(x)$ cannot be found for the directions lying in some neighborhood of the normal to the plane of L, and therefore $\rho(x)$ cannot be recovered.

The set G_τ corresponding to the complete set $\{\tau\}$ is called complete. This follows from the assertion proved above.

If the set G_τ contains diametrally opposed points, then it is complete. Such a domain can be any curve joining diametrally opposed points. In the simplest case it will be a great semicircle.

If a two-dimensional domain G_τ is complete, but does not contain diametrally opposed points, then the boundary[3] of G_τ is complete.

4. FORM OF THE VARIOUS PROJECTIONS (τ)

We now show that if the projections of $\rho(x)$ are known along some curve Γ, joining the arbitrary points P_1 and P_2 on the sphere of directions, then it is possible to determine the projection of $\rho(x)$ along the shortest curve Γ_0 of the arc of the great circle joining these points.

Let (τ_0) be an arbitrary projection lying on Γ_0, and let $\{\tau\}$ be the set of directions corresponding to Γ. Project each two-dimensional function $\rho(x, \tau)$ from the set $\{\tau\}$ along the direction $\tau_0 - \tau(\tau_0\tau)$. This projection coincides with the projection of the function $\rho(x, \tau_0)$ along the direction $\tau - \tau_0(\tau_0\tau)$, and both coincide with the convolution $\widehat{\rho(x)\delta}(x, n)$, where $n = [\tau_0\tau]\,|[\tau_0\tau]|^{-1}$, $\delta(nx) = \delta(\eta)$ being the one-dimensional δ-function. As τ moves along Γ the vector n (up to sign) runs over all possible directions in the plane perpendicular to the vector τ_0. This means that ll the projections of the two-dimensional function $\rho(x,$ $)$ are known, and therefore $\rho(x, \tau_0)$ can be recovered by adon's equation.

Let us obtain the appropriate equation. Let $\rho(x,\tau) =$ We have

$$\psi(x, [\tau_0 n]) = \int_{-\infty}^{\infty} \psi(x+[\tau_0 n]\eta)\, d\eta = \int_{-\infty}^{\infty} \rho(x+[\tau n]\eta, \tau)\, d\eta. \quad (3)$$

/ Radon's equation we obtain

$$\psi(x) = -\frac{\Delta}{2\pi^2} \int_0^{\pi} d\varphi_n \int_{-\infty}^{\infty} dt\, \psi(nt, [\tau_0 n]) \ln|t - nx|, \quad (4)$$

iere Δ is the Laplace operator. We substitute (3) in):

$$\rho(x, \tau) = -\frac{\Delta}{2\pi^2} \int_0^{\pi} d\varphi_n \int_{\Sigma_\tau} dS' \rho(x', \tau) \ln|nx' - nx|, \quad (5)$$

ere Σ_τ is the plane which passes through the coordi- :e origin and perpendicular to the vector τ. Now we press integration with respect to the azimuth of the ctor n in the form of an integral along Γ:

$$d\varphi_n = \frac{(\tau_0 \tau \dot{\tau})}{|[\tau_0 \tau]|^2} dl, \quad (6)$$

ere dl is the element of length along Γ, $\dot{\tau} = d\tau/dl$, and $\tau\dot{\tau})$ is the triple scalar product of the vectors τ_0, τ, l $\dot{\tau}$. Finally,

$$\rho(x, \tau_0) = \frac{1}{2\pi^2} \int_{P_1}^{P_2} (\tau_0 \tau \dot{\tau})\, dl \int_{\Sigma_\tau} dS' \frac{\rho(x, \tau) - \rho(x', \tau)}{(\tau_0 \tau x - x')^2}. \quad (7)$$

Now let some closed simple (nonself-intersecting) ve Γ be given on S. Consider that domain G of the ere which is bounded by Γ, and has solid angle $\Omega \leq$ with respect to the center of the sphere.

Any projection (τ_0), lying inside G can be found from known projection $\{\tau_\Gamma\}$ along the boundary of the domain. prove this, it suffices to pass an arc of a great circle ough the point $P_{\tau 0}$, where the arc meets the boundary at the points P_1 and P_2, and then to use the results ec. 4.

YMMETRY

If the object has point-symmetry group g, then the tion $\rho(x)$ is invariant with respect to the transforma- operators F_k of this group:

$$\rho(F_k x) = \rho(x) \quad (k = 1, 2, \ldots, p), \quad (8)$$

re p is the order of the group g. From this relation from the definition of the projection it follows that projections in directions forming the star of this group interrelated by the equation

$$\rho(x, F_k \tau) = \rho(F_k^{-1} x, \tau). \quad (9)$$

is assumed that the projections of the object have ral symmetry

$$\rho(x, -\tau) = \rho(x, \tau),$$

then it can be concluded that the group of symmetries of the directions of the projections of the object under consideration is obtained from g by adding the center of inversion, i.e., it is similar to the Laue class corresponding to the group g. We shall denote this group by g^L, and the corresponding operators by $F_k^L (k = 1, 2, \ldots, P_L)$. The sphere of directions S can be partitioned into P_L independent domains $G_0^{(i)}$, which are transformed into each other under the action of the operators F_k^L:

$$F_k^L G_0^{(m)} = G_0^{(i)}, \quad (10)$$

while in $G_0^{(i)}$ there are no points which are related to each other by any symmetry transformation F_k^L. The boundary of the domain G_0 is complete.

A stronger assertion can be formulated about subsets of the domain G_0, which have the completeness property. If the results of Sec. 4 are taken into account, then it suffices that only one-dimensional subsets are considered — lines on the sphere S.

Suppose that some curve Γ is given in some domain G_0. If among the operators F_k^L of the group g^L there are operators F_{mq}^L $(q = 1, 2, \ldots, s, s \leq p)$, such that the curve $\sum_{q=1}^{s} F_{mq}^L \Gamma$ is closed and encompasses a domain $\Omega \leq 2\pi$, which completely contains some domain G_0, then the curve Γ will be complete. We shall now indicate complete Γ for the various point groups which have a center of inversion. Such groups are groups of regular prisms with an n-th order axis of symmetry:

$$g = \begin{cases} n/m, & n/mmm, \text{ n is even}, \\ n, & nm, \text{ n is odd}. \end{cases}$$

and groups of regular polyhedra: the cubic groups m3, m3m, and the icosahedral group 53m.

The choice of the domain G_0 having area $4\pi/\rho$ is unique only for the high symmetry groups 53m and m3m, for which this domain is a spherical triangle. For the remaining groups the choice of the domain G_0 is to some degree arbitrary, but the independent domain can always be chosen to be a spherical triangle whose sides are great circle arcs. For example:

1) $$g = \begin{cases} n/m, & \text{n is even}, \\ n, & \text{n is odd}, \end{cases}$$

A vertex of the spherical triangle is at the point where an n axis leaves the sphere S, and its base is the arc $\Gamma_0 = 2\pi/n$ of the great circle perpendicular to the n axis.

2) $$g = \begin{cases} n/mmm, & \text{n is even}, \\ nm, & \text{n is odd}. \end{cases}$$

A vertex of the triangle is the point where the n axis leaves the sphere S, and its base is the arc $\Gamma_0 = \pi/n$ of the great circle perpendicular to the n axis. When n is even, the arc Γ_0 is located between points where the second-order axes leave the sphere S; for odd n, it is cut in two by the point where the 2 axis leaves the sphere.

3) m3, p = 24.

One vertex of the triangle is at the point where the 3 axis leaves S, and the other two are at the points where the 2 axes leave S.

4) m3m, p = 48.

The triangle is defined by the points where the 4, 3, and 2 axes leave S.

5) 53m, p = 120.

The triangle is defined by the points where the 5, 3, and 2 axes leave S.

It is easy to prove that for all the groups listed above, except for n and nm, any side of the spherical triangles so determined is complete. Also complete is any line containing some vertex of the triangle. For the groups 53m, m3m, and n/mmm, moreover, any line joining any vertex with the opposite side is complete. For the groups m3 and n/m the line joining the point where the 3 or n axis leaves the sphere with the opposite side is complete.

For the group nm those lines are complete which join the vertices of the triangle with the 2 axis, and for the group n the arc $\Gamma_0 = 2\pi/n$ of the great circle perpendicular to the n axis is complete. Any two-dimensional domain containing the complete curves Γ listed above is complete.

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[1] If the sets $\{\tau\}$ and $\{-\tau\}$ pass continuously from one to the other, then we will take $\{\tau\}$ to mean the set $\{\tau\} + \{-\tau\}$. In the opposite case, the set $\{\tau\}$ does not contain vectors which differ only by sign.

[2] A domain is any continuous connected two-dimensional or one-dimensional set of points on the sphere. A closed domain is, as usual, the union of the set and its frontier.

[3] When G_τ is multiply connected, that boundary is complete which is closest to the domain $G-\tau$, which is the image of the set $\{-\tau\}$.

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