Finding degeneracy in fluorescence orientation microscopes

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Consider a microscope with an angular point spread function $h_i(\hat{\mathbf{s}})$—we're assuming that the spatial and angular problems are decoupled. The forward model for this microscope is

$$g_i = \int_{\mathbb{S}^2} d\hat{\mathbf{s}}\, h_i(\hat{\mathbf{s}}) f(\hat{\mathbf{s}}), \qquad i = 1, 2, ..., N. \tag{1}$$

where $f(\hat{\mathbf{s}})$ is the angular density of fluorophores and i indexes N measurements.

We would like to find the angular degeneracies of this microscope. In other words, what rotations $\mathbf{R}$ can we apply to samples $f(\hat{\mathbf{s}})$ and measure the same data? Mathematically, we need to find the set of matrices $\mathbf{R}$ and functions $f(\hat{\mathbf{s}})$ that satisfy

$$\int_{\mathbb{S}^2} d\hat{\mathbf{s}}\, h_i(\hat{\mathbf{s}}) f(\hat{\mathbf{s}}) - \int_{\mathbb{S}^2} d\hat{\mathbf{s}}\, h_i(\hat{\mathbf{s}}) f(\mathbf{R}^{-1}\hat{\mathbf{s}}) = 0, \qquad i = 1, 2, ..., N. \tag{2}$$

We will start by restricting the problem to objects where all of the fluorophores are oriented in the same direction so that $f(\hat{\mathbf{s}}) = \delta(\hat{\mathbf{s}} - \hat{\mathbf{s}}_1)$. In this case we need to find the set of directions $\hat{\mathbf{s}}_1$ and matrices $\mathbf{R}$ that satisfy

$$h_i(\hat{\mathbf{s}}_1) - h_i(\mathbf{R}^{-1}\hat{\mathbf{s}}_1) = 0, \qquad i = 1, 2, ..., N. \tag{3}$$

We have a set of N equations that we need to solve simultaneously for $\hat{\mathbf{s}}_1 \in \mathbb{S}^2$ and $\mathbf{R} \in \mathbb{SO}(3)$. As far as I can tell there is no analytic way to solve this set of equations in the general case. I tried expanding onto spherical and rotational harmonics, but that didn't help because there's no easy way to relate a solution in the frequency domain to a solution in the normal domain. Instead, we can find as many solutions as we can "by hand" then check our results numerically. I've used optimization packages the can optimize on $\mathbb{S}^2 \times \mathbb{SO}(3)$—my rough plan is to seed an optimization procedure at many place on a grid in $\mathbb{S}^2 \times \mathbb{SO}(3)$ and check (not prove!) that we have all of the solutions with those results. Other ideas welcome!

For now let's solve a simple case "by hand". If we have a single point detector along the z axis then our angular point spread function is given by

$$h^{(\hat{\mathbf{z}})}(\hat{\mathbf{s}}_1) = 1 - (\hat{\mathbf{s}}_1 \cdot \hat{\mathbf{z}})^2. \tag{4}$$

This is the first time I'm expressing an angular point spread function in vector notation, but it's easy to check that this reduces to the familiar $h^{(\hat{\mathbf{z}})}(\hat{\mathbf{s}}_1) = \sin^2\vartheta$ if you choose spherical coordinates so that $\hat{\mathbf{s}}_1 = \cos\varphi\sin\vartheta\hat{\mathbf{x}} + \sin\varphi\sin\vartheta\hat{\mathbf{y}} + \cos\vartheta\hat{\mathbf{z}}$. Plugging Eq. 4 into Eq. 2 gives

$$-(\hat{\mathbf{s}}_1 \cdot \hat{\mathbf{z}})^2 + (\mathbf{R}^{-1}\hat{\mathbf{s}}_1 \cdot \hat{\mathbf{z}})^2 = 0. \tag{5}$$

I can find the following solutions to this equation for all $\hat{\mathbf{s}}_1 \in \mathbb{S}^2$

$$\mathbf{R}_0 = \begin{bmatrix} \cos\theta & -\sin\theta & 0 \\ \sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{bmatrix} \text{ for } 0 \leq \theta < 2\pi, \tag{6}$$

which is an arbitrary rotation about the z axis;

$$\mathbf{R}_1 = \mathbf{I} + 2\,[\mathbf{k}]_\times^2 \tag{7}$$

where

$$\mathbf{k} = \frac{\hat{\mathbf{s}}_1 \times [(\hat{\mathbf{s}}_1 \cdot \hat{\mathbf{z}})\hat{\mathbf{z}}]}{|\hat{\mathbf{s}}_1 \times [(\hat{\mathbf{s}}_1 \cdot \hat{\mathbf{z}})\hat{\mathbf{z}}]|}, \qquad [\mathbf{k}]_\times = \begin{bmatrix} 0 & -k_z & k_y \\ k_z & 0 & -k_x \\ -k_y & k_x & 0 \end{bmatrix}, \tag{8}$$

which is a rotation that maps $\hat{\mathbf{s}}_1$ to $-\hat{\mathbf{s}}_1$; and

$$\mathbf{R}_2 = \mathbf{I} + 2(\hat{\mathbf{s}}_1 \cdot \hat{\mathbf{z}})\sqrt{1 - (\hat{\mathbf{s}}_1 \cdot z)^2}\,[\mathbf{k}]_\times + 2(\hat{\mathbf{s}}_1 \cdot \hat{\mathbf{z}})^2\,[\mathbf{k}]_\times^2 \tag{9}$$

which is a rotation that maps every $\hat{\mathbf{s}}_1$ above the $x - y$ plane to an $\hat{\mathbf{s}}_1$ below the $x - y$ plane and vice versa. Notice that

$$\mathbf{R}_3 = \begin{bmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{bmatrix} \tag{10}$$

is not a solution because $\mathbf{R}_3$ is not a member of $\mathbb{SO}(3)$—$\mathbf{R}_3$ is a member of the larger set $\mathbb{O}(3)$. This distinction is important so that we don't double count solutions.

We can identify the solutions $\mathbf{R}_0$, $\mathbf{R}_1$, and $\mathbf{R}_2$ as matrix representations of a group. This group is a *Frieze group* with *dihedral symmetry*, an infinite number of possible rotations, and a horizontal reflection axis. Using Schönflies notation we say that $D_{\infty h}$ is the symmetry group of the imaging system.