Singular value decomposition of single view polarized fluorescence microscopes

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1 Introduction

In these notes we will develop the continuous models for single view polarized fluorescence microscopes with either polarized illumination or polarized detection. We will start by writing an integral transform that maps object space to data space. Then we will calculate the kernels of the integral transform and their corresponding transfer functions. Finally we will calculate the singular value decomposition of the forward operator to find the limits of these designs.

We will make use of the real circular harmonic functions

$$z_n(\theta) = \begin{cases} \frac{1}{\sqrt{\pi}}\cos(n\theta), & n > 0, \\ \frac{1}{\sqrt{2\pi}}, & n = 0, \\ \frac{1}{\sqrt{\pi}}\sin(n\theta), & n < 0. \end{cases} \tag{1}$$

The real circular harmonic functions form an orthonormal basis for functions on the circle because

$$\int_{\mathbb{S}^1} d\hat{\mathbf{p}}\, z_n(\hat{\mathbf{p}}) z_{n'}(\hat{\mathbf{p}}) = \delta_{nn'}. \tag{2}$$

Notice that we allow $z_n(\cdot)$ to take a vector argument similar to the spherical harmonics $y_l^m(\hat{\mathbf{s}}_o)$. This allows us to use these functions without specifying a coordinate system. Also notice that we are using n to index the circular harmonic functions—in a previous note set we used n to index frames or views.

2 General forward model

We will consider the problem of imaging a two-dimensional field of oriented fluorophores. To a good approximation these objects can be represented by a member of the set $\mathbb{U} = \mathbb{L}_2(\mathbb{R}^2 \times \mathbb{S}^2)$—square-integrable functions that assign a scalar value to each position and orientation.

These microscopes can collect a two-dimensional frame of intensity measurements for each position of a single polarizer on the illumination or detection arm. Therefore, the collected data is a member of the set $\mathbb{V} = \mathbb{L}_2(\mathbb{R}^2 \times \mathbb{S}^1)$—square-integrable functions that assign a scalar value to each two-dimensional position on a circle. Notice that we are considering the largest possible data space for these microscopes—a continuous sampling of the spatial and polarizer dimensions. This approach allows us to answer questions about the limits of these microscopes without considering specific choices of spatial sampling (pixels) or polarization sampling (polarizer settings). It will be helpful to think of the space $\mathbb{L}_2(\mathbb{R}^2 \times \mathbb{S}^1)$ geometrically as a continuous list of images arranged face to face in a donut—if we slice the donut along the smaller dimension (not like a pre-cut bagel!) we can see a single image taken with a single polarizer setting.

If the imaging system is spatially shift-invariant, then the forward and adjoint operators are given by the following integral transforms

$$g(\mathbf{r}_d, \hat{\mathbf{p}}) = [\mathcal{H}f](\mathbf{r}_d, \hat{\mathbf{p}}) = \int_{\mathbb{S}^2} d\hat{\mathbf{s}}_o \int_{\mathbb{R}^2} d\mathbf{r}_o\, h(\mathbf{r}_d - \mathbf{r}_o, \hat{\mathbf{s}}_o; \hat{\mathbf{p}}) f(\mathbf{r}_o, \hat{\mathbf{s}}_o), \tag{3}$$

$$f(\mathbf{r}_o, \hat{\mathbf{s}}_o) = [\mathcal{H}^\dagger g](\mathbf{r}_o, \hat{\mathbf{s}}_o) = \int_{\mathbb{S}^1} d\hat{\mathbf{p}} \int_{\mathbb{R}^2} d\mathbf{r}_d\, h(\mathbf{r}_d - \mathbf{r}_o, \hat{\mathbf{s}}_o; \hat{\mathbf{p}}) g(\mathbf{r}_d, \hat{\mathbf{p}}). \tag{4}$$

where $f(\mathbf{r}_o, \hat{\mathbf{s}}_o)$ is the object, $g(\mathbf{r}_d, \hat{\mathbf{p}})$ is the data, and $h(\mathbf{r}_d - \mathbf{r}_o, \hat{\mathbf{s}}_o; \hat{\mathbf{p}})$ is the kernel of the integral transform. The kernel can be interpreted as a "point spread function" if we visualize the complete data space as a "donut" of images. A delta function at a point in object space will give rise to the kernel evaluated at that point in data space.

We can write the forward and adjoint operators in the frequency domain as

$$G_n(\boldsymbol{\nu}) = \sum_{l=0}^{\infty}\sum_{m=-l}^{l} H_{l,n}^m(\boldsymbol{\nu})F_l^m(\boldsymbol{\nu}), \tag{5}$$

$$F_l^m(\boldsymbol{\nu}) = \sum_{n=-\infty}^{\infty} H_{l,n}^m(\boldsymbol{\nu})G_n(\boldsymbol{\nu}), \tag{6}$$

where

$$G_n(\boldsymbol{\nu}) = \int_{\mathbb{S}^1} d\hat{\mathbf{p}}\, z_n(\hat{\mathbf{p}}) \int_{\mathbb{R}^2} d\mathbf{r}_d\, \mathrm{e}^{i2\pi\mathbf{r}_d\cdot\boldsymbol{\nu}} g(\mathbf{r}_d, \hat{\mathbf{p}}), \tag{7}$$

$$H_{l,n}^m(\boldsymbol{\nu}) = \int_{\mathbb{S}^1} d\hat{\mathbf{p}}\, z_n(\hat{\mathbf{p}}) \int_{\mathbb{S}^2} d\hat{\mathbf{s}}_o\, y_l^m(\hat{\mathbf{s}}_o) \int_{\mathbb{R}^2} d\mathbf{r}_o\, \mathrm{e}^{i2\pi\mathbf{r}_o\cdot\boldsymbol{\nu}} h(\mathbf{r}_o, \hat{\mathbf{s}}_o; \hat{\mathbf{p}}), \tag{8}$$

$$F_l^m(\boldsymbol{\nu}) = \int_{\mathbb{S}^2} d\hat{\mathbf{s}}_o\, y_l^m(\hat{\mathbf{s}}_o) \int_{\mathbb{R}^2} d\mathbf{r}_o\, \mathrm{e}^{i2\pi\mathbf{r}_o\cdot\boldsymbol{\nu}} f(\mathbf{r}_o, \hat{\mathbf{s}}_o). \tag{9}$$

To find the singular value decomposition of the forward operator, we need to solve

$$\mathcal{H}\mathcal{H}^\dagger v_{\boldsymbol{\rho},j}(\mathbf{r}_d, \hat{\mathbf{p}}) = \mu_{\boldsymbol{\rho},j} v_{\boldsymbol{\rho},j}(\mathbf{r}_d, \hat{\mathbf{p}}). \tag{10}$$

It is much easier to solve the equivalent problem in the frequency domain

$$\mathsf{K}(\boldsymbol{\rho})\mathsf{V}_j(\boldsymbol{\rho}) = \mu_{\boldsymbol{\rho},j}\mathsf{V}_j(\boldsymbol{\rho}). \tag{11}$$

where the entries of $\mathsf{K}(\boldsymbol{\rho})$ are given by

$$K_{nn'}(\boldsymbol{\rho}) = \sum_{l=0}^{\infty}\sum_{m=-l}^{l} H_{l,n}^m(\boldsymbol{\rho})H_{l,n'}^m(\boldsymbol{\rho}), \tag{12}$$

and the entries of $\mathsf{V}_j(\boldsymbol{\rho})$ are related to the complete data space singular functions by

$$v_{\boldsymbol{\rho},j}(\mathbf{r}_d, \hat{\mathbf{p}}) = \mathrm{e}^{i2\pi\boldsymbol{\rho}\cdot\mathbf{r}_d} \sum_{n=-\infty}^{\infty} [V_n(\boldsymbol{\rho})]_j z_n(\hat{\mathbf{p}}). \tag{13}$$

Once we've found the data space singular functions, we can find the object space singular functions using

$$[U_l^m(\boldsymbol{\rho})]_j = \sum_{n=-\infty}^{\infty} H_{l,n}^m(\boldsymbol{\rho})[V_n(\boldsymbol{\rho})]_j, \tag{14}$$

$$u_{\boldsymbol{\rho},j}(\mathbf{r}_o, \hat{\mathbf{s}}_o) = \mathrm{e}^{i2\pi\boldsymbol{\rho}\cdot\mathbf{r}_o} \sum_{l=0}^{\infty}\sum_{m=-l}^{l} [U_l^m(\boldsymbol{\rho})]_j y_l^m(\hat{\mathbf{s}}_o). \tag{15}$$

3 Polarized illumination

3.1 Kernel

In previous notes we showed that the excitation point response function for polarized epi-illumination is given by

$$h_{\text{exc}}^{\hat{\mathbf{z}}}(\hat{\mathbf{s}}_o; \hat{\mathbf{p}}) = y_0^0(\hat{\mathbf{s}}_o) - \frac{1}{\sqrt{5}}\tilde{A}y_2^0(\hat{\mathbf{s}}_o) + \sqrt{\frac{3}{5}}\tilde{B}\left\{[(\hat{\mathbf{p}}\cdot\hat{\mathbf{x}})^2 - (\hat{\mathbf{p}}\cdot\hat{\mathbf{y}})^2]y_2^2(\hat{\mathbf{s}}_o) - 2(\hat{\mathbf{p}}\cdot\hat{\mathbf{x}})(\hat{\mathbf{p}}\cdot\hat{\mathbf{y}})y_2^{-2}(\hat{\mathbf{s}}_o)\right\}, \tag{16}$$

where

$$\tilde{A} \equiv \cos^2(\alpha/2)\cos(\alpha), \tag{17a}$$

$$\tilde{B} \equiv \frac{1}{12}(\cos^2\alpha + 4\cos\alpha + 7), \tag{17b}$$

and $\alpha \equiv \arcsin(\text{NA}/n_o)$. It is more convenient to write the point response function in terms of the circular harmonics

$$h_{\text{exc}}^{\hat{\mathbf{z}}}(\hat{\mathbf{s}}_o; \hat{\mathbf{p}}) = y_0^0(\hat{\mathbf{s}}_o) - \frac{1}{\sqrt{5}}\tilde{A}y_2^0(\hat{\mathbf{s}}_o) + \sqrt{\frac{3}{5}}\tilde{B}\left\{y_2^2(\hat{\mathbf{s}}_o)z_2(\hat{\mathbf{p}}) - y_2^{-2}(\hat{\mathbf{s}}_o)z_{-2}(\hat{\mathbf{p}})\right\}. \tag{18}$$

We also showed that the point response function for unpolarized epi-detection is given by

$$h_{\text{det}}(\mathbf{r}_o, \hat{\mathbf{s}}_o) = [a^2(r_o) + 2b^2(r_o)]y_0^0(\hat{\mathbf{s}}_o) + \frac{1}{\sqrt{5}}\left[-a^2(r_o) + 4b^2(r_o)\right]y_2^0(\hat{\mathbf{s}}_o), \tag{19}$$

where

$$a(r_o) = \frac{J_1(2\pi\nu_o r_o)}{\pi\nu_o r_o}, \qquad b(r_o) = \frac{\text{NA}}{n_o}\left[\frac{J_2(2\pi\nu_o r_o)}{\pi\nu_o r_o}\right], \tag{20}$$

and

$$\nu_o \equiv \frac{\text{NA}}{\lambda}, \qquad \text{NA} = n_o\sin\alpha. \tag{21}$$

The excitation and detection processes are incoherent, so to find the complete point response function we can multiply the excitation and detection point response functions which gives

$$h(\mathbf{r}_o, \hat{\mathbf{s}}_o; \hat{\mathbf{p}}) = h_{\text{exc}}^{\hat{\mathbf{z}}}(\hat{\mathbf{s}}_o; \hat{\mathbf{p}})h_{\text{det}}(\mathbf{r}_o, \hat{\mathbf{s}}_o) = \frac{1}{\tilde{N}}\sum_{l=0}^{\infty}\sum_{m=-l}^{l}\sum_{n=-\infty}^{\infty} h_{l,n}^m(\mathbf{r}_o)y_l^m(\hat{\mathbf{s}}_o)z_n(\hat{\mathbf{p}}), \tag{22}$$

where $\tilde{N} = \frac{\tilde{A}}{10} + \frac{1}{2}$ is a normalization constant and the terms in the series are given by

$$h_{0,0}^0(r_o) = \left[\frac{\tilde{A}}{10} + \frac{1}{2}\right]a^2(r_o) + \left[-\frac{2\tilde{A}}{5} + 1\right]b^2(r_o), \tag{23}$$

$$h_{2,2}^2(r_o) = -h_{2,-2}^{-2}(r_o) = \frac{3\sqrt{15}\tilde{B}}{35}\left[\frac{3}{2}a^2(r_o) + b^2(r_o)\right], \tag{24}$$

$$h_{2,0}^0(r_o) = \left[-\frac{\sqrt{5}\tilde{A}}{14} + \frac{\sqrt{5}}{10}\right]a^2(r_o) + \left[-\frac{11\sqrt{5}\tilde{A}}{35} + \frac{2}{\sqrt{5}}\right]b^2(r_o), \tag{25}$$

$$h_{4,2}^2(r_o) = -h_{4,-2}^{-2}(r_o) = \frac{6\sqrt{5}\tilde{B}}{35}\left[-\frac{1}{4}a^2(r_o) + b^2(r_o)\right], \tag{26}$$

$$h_{4,0}^0(r_o) = \frac{3\tilde{A}}{35}[a^2(r_o) - 4b^2(r_o)], \tag{27}$$

$$\tag{28}$$

and all other $h_{l,n}^m(r_o)$ terms in the series are zero.

3.2 Transfer function

The optical transfer function for this microscope is given by

$$H_{l,n}^{m}(\nu) = \frac{1}{\tilde{M}} \sum_{l'=0}^{\infty} \sum_{m'=-l'}^{l'} \sum_{n'=-\infty}^{\infty} H_{l',n'}^{m'}(\nu)\delta_{l,l'}\delta_{m,m'}\delta_{n,n'}, \tag{29}$$

where $\tilde{M} = \left[\frac{\tilde{A}}{10} + \frac{1}{2}\right] + \left(\frac{\text{NA}}{n_o}\right)\left[-\frac{2\tilde{A}}{10} + \frac{1}{2}\right]$ is a normalization constant, and

$$H_{0,0}^{0}(\nu) = \left[\frac{\tilde{A}}{10} + \frac{1}{2}\right] A(\nu) + \left[-\frac{2\tilde{A}}{5} + 1\right] B(\nu), \tag{30}$$

$$H_{2,2}^{2}(\nu) = -H_{2,-2}^{-2}(\nu) = \frac{3\sqrt{15}\tilde{B}}{35}\left[\frac{3}{2}A(\nu) + B(\nu)\right], \tag{31}$$

$$H_{2,0}^{0}(\nu) = \left[-\frac{\sqrt{5}\tilde{A}}{14} + \frac{\sqrt{5}}{10}\right] A(\nu) + \left[-\frac{11\sqrt{5}\tilde{A}}{35} + \frac{2}{\sqrt{5}}\right] B(\nu), \tag{32}$$

$$H_{4,2}^{2}(\nu) = -H_{4,-2}^{-2}(\nu) = \frac{6\sqrt{5}\tilde{B}}{35}\left[-\frac{1}{4}A(\nu) + B(\nu)\right], \tag{33}$$

$$H_{4,0}^{0}(\nu) = \frac{3\tilde{A}}{35}[A(\nu) - 4B(\nu)], \tag{34}$$

and all other $H_{l,n}^{m}(\nu)$ terms in the series are zero, and

$$A(\nu) = \frac{2}{\pi}\left[\arccos\left(\frac{\nu}{2\nu_o}\right) - \frac{\nu}{2\nu_o}\sqrt{1 - \left(\frac{\nu}{2\nu_o}\right)^2}\right]\Pi\left(\frac{\nu}{2\nu_o}\right), \tag{35}$$

$$B(\nu) = \frac{1}{\pi}\left(\frac{\text{NA}}{n_o}\right)^2\left[\arccos\left(\frac{\nu}{2\nu_o}\right) - \left[3 - 2\left(\frac{\nu}{2\nu_o}\right)^2\right]\frac{\nu}{2\nu_o}\sqrt{1 - \left(\frac{\nu}{2\nu_o}\right)^2}\right]\Pi\left(\frac{\nu}{2\nu_o}\right). \tag{36}$$

3.3 Singular value decomposition

Plugging the transfer function into the frequency-domain eigenvalue problem (Eq. 11) yields a 3×3 eigenvalue problem (we suppress the index $\boldsymbol{\rho}$ and understand that we need to solve this eigenvalue problem at each value of $\boldsymbol{\rho}$)

$$\mathsf{K}\mathsf{V}_j = \mu_j \mathsf{V}_j, \tag{37}$$

$$\begin{bmatrix} \sum_{l,m} H_{l,-2}^{m} H_{l,-2}^{m} & \sum_{l,m} H_{l,-2}^{m} H_{l,0}^{m} & \sum_{l,m} H_{l,-2}^{m} H_{l,2}^{m} \\ \sum_{l,m} H_{l,0}^{m} H_{l,-2}^{m} & \sum_{l,m} H_{l,0}^{m} H_{l,0}^{m} & \sum_{l,m} H_{l,0}^{m} H_{l,2}^{m} \\ \sum_{l,m} H_{l,2}^{m} H_{l,-2}^{m} & \sum_{l,m} H_{l,2}^{m} H_{l,0}^{m} & \sum_{l,m} H_{l,2}^{m} H_{l,2}^{m} \end{bmatrix} \mathsf{V}_j = \mu_j \mathsf{V}_j, \tag{38}$$

$$\begin{bmatrix} \{H_{2,-2}^{-2}\}^2 + \{H_{4,-2}^{-2}\}^2 & 0 & 0 \\ 0 & \{H_{0,0}^{0}\}^2 + \{H_{2,0}^{0}\}^2 + \{H_{4,0}^{0}\}^2 & 0 \\ 0 & 0 & \{H_{2,2}^{2}\}^2 + \{H_{4,2}^{2}\}^2 \end{bmatrix} \mathsf{V}_j = \mu_j \mathsf{V}_j. \tag{39}$$

A diagonal matrix has its eigenvalues along the diagonal and its eigenvectors as unit vectors so

$$\mu_{\boldsymbol{\rho},0} = \{H_{0,0}^{0}(\rho)\}^2 + \{H_{2,0}^{0}(\rho)\}^2 + \{H_{4,0}^{0}(\rho)\}^2, \tag{40}$$

$$\mu_{\boldsymbol{\rho},1} = \mu_{\boldsymbol{\rho},2} = \{H_{2,2}^{2}(\rho)\}^2 + \{H_{4,2}^{2}(\rho)\}^2, \tag{41}$$

and

$$\mathsf{V}_0 = \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix}, \qquad \mathsf{V}_1 = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}, \qquad \mathsf{V}_2 = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}. \tag{42}$$

Notice that we have two degenerate eigenvalues, but we have found trivial orthonormal eigenvectors—in general we will need to apply the Gram-Schmidt procedure.

We can use Eq. 13 to recover the complete singular functions in data space as

$$v_{\boldsymbol{\rho},0}(\mathbf{r}_d, \hat{\mathbf{p}}) = \mathrm{e}^{i2\pi\boldsymbol{\rho}\cdot\mathbf{r}_d} z_0(\hat{\mathbf{p}}), \tag{43}$$
$$v_{\boldsymbol{\rho},1}(\mathbf{r}_d, \hat{\mathbf{p}}) = \mathrm{e}^{i2\pi\boldsymbol{\rho}\cdot\mathbf{r}_d} z_{-2}(\hat{\mathbf{p}}), \tag{44}$$
$$v_{\boldsymbol{\rho},2}(\mathbf{r}_d, \hat{\mathbf{p}}) = \mathrm{e}^{i2\pi\boldsymbol{\rho}\cdot\mathbf{r}_d} z_2(\hat{\mathbf{p}}). \tag{45}$$

For the final step we use Eq. 14 to find the spectra of the singular functions in object space

$$[U_l^m(\rho)]_0 = H_{l,0}^m(\rho) = H_{0,0}^0(\rho)\delta_{l0}\delta_{m0} + H_{2,0}^0(\rho)\delta_{l2}\delta_{m0} + H_{4,0}^0(\rho)\delta_{l4}\delta_{m0}, \tag{46}$$
$$[U_l^m(\rho)]_1 = H_{l,-2}^m(\rho) = H_{2,-2}^{-2}(\rho)\delta_{l2}\delta_{m-2} + H_{4,-2}^{-2}(\rho)\delta_{l4}\delta_{m-2}, \tag{47}$$
$$[U_l^m(\rho)]_2 = H_{l,2}^m(\rho) = H_{l,2}^m(\rho) = H_{2,2}^2(\rho)\delta_{l2}\delta m2 + H_{4,2}^2(\rho)\delta_{l4}\delta_{m2}. \tag{48}$$

Therefore, the complete singular functions in object space are

$$u_{\boldsymbol{\rho},0}(\mathbf{r}_o, \hat{\mathbf{s}}_o) = \mathrm{e}^{i2\pi\boldsymbol{\rho}\cdot\mathbf{r}_o}[H_{0,0}^0(\rho)y_0^0(\hat{\mathbf{s}}_o) + H_{2,0}^0(\rho)y_2^0(\hat{\mathbf{s}}_o) + H_{4,0}^0(\rho)y_4^0(\hat{\mathbf{s}}_o)], \tag{49}$$
$$u_{\boldsymbol{\rho},1}(\mathbf{r}_o, \hat{\mathbf{s}}_o) = \mathrm{e}^{i2\pi\boldsymbol{\rho}\cdot\mathbf{r}_o}[H_{2,-2}^{-2}(\rho)y_2^{-2}(\hat{\mathbf{s}}_o) + H_{4,-2}^{-2}(\rho)y_4^{-2}(\hat{\mathbf{s}}_o)], \tag{50}$$
$$u_{\boldsymbol{\rho},2}(\mathbf{r}_o, \hat{\mathbf{s}}_o) = \mathrm{e}^{i2\pi\boldsymbol{\rho}\cdot\mathbf{r}_o}[H_{2,2}^2(\rho)y_2^2(\hat{\mathbf{s}}_o) + H_{4,2}^2(\rho)y_4^2(\hat{\mathbf{s}}_o)]. \tag{51}$$

We have found the complete singular system for a single view microscope with polarized illumination. We can look closer at the singular value spectrum to find the degeneracies of the microscope. The first major set of degeneracies is related to the fact that $\mu_{\boldsymbol{\rho},1} = \mu_{\boldsymbol{\rho},2}$. The corresponding singular functions in object space are related by changing the spherical harmonic index m to $-m$. This transformation is a rotation about the optical axis, so this degeneracy corresponds to the rotational symmetry of the microscope. The second set of degeneracies is related to the fact that the singular values depend only on ρ, not the vector $\boldsymbol{\rho}$. The corresponding singular functions in object space are spatial harmonics at the same spatial frequency in different directions. Once again, this degeneracy corresponds to the rotational symmetry of the microscope.

Recall the mental image of data space being arranged on a donut. If we rotate the object that we are imaging then the data space will undergo two simultaneous rotations—one rotation about an axis through the donut hole (imagine sticking your finger through the donut) and another about the curved axis that runs through the center of the dough (imagine twisting the donut in on itself so that glaze on top would end up on the bottom). These two simultaneous rotations correspond with the two sets of degeneracies we see in the singular value spectrum.

Plots forthcoming!

4 Polarized detection

We'll use the same notation as the previous section, so there will be notation overlap.

4.1 Kernel

In previous notes we showed that the excitation point response function for unpolarized epi-illumination is given by

$$h_{\text{exc}}^{\hat{\mathbf{z}}}(\hat{\mathbf{s}}_o) = h_{\text{exc},0,0}^0 y_0^0(\hat{\mathbf{s}}_o) + h_{\text{exc},0,0}^2 y_2^0(\hat{\mathbf{s}}_o). \tag{52}$$

where

$$h^0_{\text{exc},0,0} = 1, \tag{53}$$

$$h^0_{\text{exc},2,0} = -\frac{1}{\sqrt{5}}\tilde{A}. \tag{54}$$

We also showed that the point response function for polarized detection is given by (rewritten in terms of the circular harmonics)

$$h_{\text{det}}(\mathbf{r}_o, \hat{\mathbf{s}}_o; \hat{\mathbf{p}}) = \sum_{l=0}^{\infty}\sum_{m=-l}^{l}\sum_{n=-\infty}^{\infty} h^m_{\text{det},l,n}(\mathbf{r}_o) y^m_l(\hat{\mathbf{s}}_o) z_n(\hat{\mathbf{p}}_d), \tag{55}$$

where

$$h^0_{\text{det},0,0}(\mathbf{r}_o) = a^2(r_o) + 2b^2(r_0), \tag{56}$$

$$h^0_{\text{det},0,\pm2}(\mathbf{r}_o) = 2\sqrt{\pi}b^2(r_0)z_{\pm2}(\mathbf{r}_o), \tag{57}$$

$$h^0_{\text{det},2,0}(\mathbf{r}_o) = \frac{1}{\sqrt{5}}\left[-a^2(r_o) + 4b^2(r_0)\right], \tag{58}$$

$$h^0_{\text{det},2,\pm2}(\mathbf{r}_o) = 4\sqrt{\frac{\pi}{5}}b^2(r_0)z_{\pm2}(\mathbf{r}_o), \tag{59}$$

$$h^2_{\text{det},2,2}(\mathbf{r}_o) = -h^{-2}_{\text{det},2,-2}(\mathbf{r}_o) = \sqrt{\frac{3}{5}}a^2(r_o). \tag{60}$$

The complete kernel for unpolarized illumination and polarized detection is given by the product of the excitation and detection kernels. In the previous case we were able to calculate this product in terms of the circular and spherical harmonics by hand, but this task is difficult in the general case. To simplify this task we precompute the triple integrals of the circular and spherical harmonics—see Appendix A for details.

$$h(\mathbf{r}_o, \hat{\mathbf{s}}_o; \hat{\mathbf{p}}_d) = h_{\text{exc}}(\hat{\mathbf{s}}_o)h_{\text{det}}(\mathbf{r}_o, \hat{\mathbf{s}}_o; \hat{\mathbf{p}}_d) = \sum_{l=0}^{\infty}\sum_{m=-l}^{l}\sum_{n=-\infty}^{\infty} h^m_{l,n}(\mathbf{r}_o) y^m_l(\hat{\mathbf{s}}_o) z_n(\hat{\mathbf{p}}_d), \tag{61}$$

where

$$h^0_{0,0}(\mathbf{r}_o) = h^0_{\text{exc},0,0}h^0_{\text{det},0,0}(\mathbf{r}_o) + h^0_{\text{exc},2,0}h^0_{\text{det},2,0}(\mathbf{r}_o), \tag{62}$$

$$h^0_{0,\pm2}(\mathbf{r}_o) = h^0_{\text{exc},0,0}h^0_{\text{det},0,\pm2}(\mathbf{r}_o) + h^0_{\text{exc},2,0}h^0_{\text{det},2,\pm2}(\mathbf{r}_o), \tag{63}$$

$$h^0_{2,0}(\mathbf{r}_o) = h^0_{\text{exc},0,0}h^0_{\text{det},0,0}(\mathbf{r}_o) + h^0_{\text{exc},2,0}h^0_{\text{det},2,0}(\mathbf{r}_o) + \frac{2\sqrt{5}}{7}h^0_{\text{exc},2,0}h^0_{\text{det},2,0}(\mathbf{r}_o), \tag{64}$$

$$h^0_{2,\pm2}(\mathbf{r}_o) = h^0_{\text{exc},0,0}h^0_{\text{det},0,\pm2}(\mathbf{r}_o) + h^0_{\text{exc},2,0}h^0_{\text{det},2,\pm2}(\mathbf{r}_o) + \frac{2\sqrt{5}}{7}h^0_{\text{exc},2,0}h^0_{\text{det},2,\pm2}(\mathbf{r}_o), \tag{65}$$

$$h^{\pm2}_{2,\pm2}(\mathbf{r}_o) = h^{\pm2}_{\text{det},2,\pm2}(\mathbf{r}_o)\left[h^0_{\text{exc},0,0} - \frac{2\sqrt{5}}{7}h^0_{\text{exc},2,0}\right], \tag{66}$$

$$h^0_{4,0}(\mathbf{r}_o) = \frac{6}{7}h^0_{\text{exc},2,0}h^0_{\text{det},2,0}(\mathbf{r}_o), \tag{67}$$

$$h^0_{4,\pm2}(\mathbf{r}_o) = \frac{6}{7}h^0_{\text{exc},2,0}h^0_{\text{det},2,\pm2}(\mathbf{r}_o), \tag{68}$$

$$h^{\pm2}_{4,\pm2}(\mathbf{r}_o) = \frac{\sqrt{15}}{7}h^0_{\text{exc},2,0}h^{\pm2}_{\text{det},2,\pm2}(\mathbf{r}_o), \tag{69}$$

and the remaining terms in the series are zero. Plugging in the excitation and detection point response functions gives the following

$$h^0_{0,0}(\mathbf{r}_o) = \left[\frac{\tilde{A}}{5}+1\right] a^2(r_o) + \left[-\frac{4\tilde{A}}{5}+2\right] b^2(r_o), \tag{70}$$

$$h^0_{0,\pm2}(\mathbf{r}_o) = 2\sqrt{\pi}\left[1-\frac{2\tilde{A}}{5}\right] b^2(r_o) z_{\pm2}(\mathbf{r}_o), \tag{71}$$

$$h^0_{2,0}(\mathbf{r}_o) = \frac{\sqrt{5}}{35}\left\{-\left[5\tilde{A}+7\right] a^2(r_o) + \left[-22\tilde{A}+28\right] b^2(r_0)\right\}, \tag{72}$$

$$h^0_{2,\pm2}(\mathbf{r}_o) = \frac{2\sqrt{5\pi}}{35}\left[-11\tilde{A}+14\right] b^2(r_o) z_{\pm2}(\mathbf{r}_o) \tag{73}$$

$$h^2_{2,2}(\mathbf{r}_o) = h^{-2}_{2,-2}(\mathbf{r}_o) = \frac{\sqrt{15}}{5}\left[\frac{2\tilde{A}}{7}+1\right] a^2(r_o), \tag{74}$$

$$h^0_{4,0}(\mathbf{r}_o) = \frac{6\tilde{A}}{35}\left[a^2(r_o) - 4b^2(r_o)\right], \tag{75}$$

$$h^0_{4,\pm2}(\mathbf{r}_o) = -\frac{24\sqrt{\pi}}{35}\tilde{A} b^2(r_o) z_{\pm2}(\mathbf{r}_o), \tag{76}$$

$$h^2_{4,2}(\mathbf{r}_o) = h^{-2}_{4,-2}(\mathbf{r}_o) = -\frac{3\sqrt{5}}{35}\tilde{A} a^2(r_o). \tag{77}$$

4.2 Transfer function

The transfer function for unpolarized illumination and polarized detection is given by

$$H^m_{l,n}(\boldsymbol{\nu}) = \sum_{l=0}^{\infty}\sum_{m=-l}^{l}\sum_{n=-\infty}^{\infty} H^m_{l,n}(\boldsymbol{\nu})\delta_{ll'}\delta_{mm'}\delta_{nn'}, \tag{78}$$

where

$$H^0_{0,0}(\boldsymbol{\nu}) = \left[\frac{\tilde{A}}{5}+1\right] A(\nu) + \left[-\frac{4\tilde{A}}{5}+2\right] B(\nu), \tag{79}$$

$$H^0_{0,\pm2}(\boldsymbol{\nu}) = 2\sqrt{\pi}\left[1-\frac{2\tilde{A}}{5}\right] C(\nu) z_{\pm2}(\boldsymbol{\nu}), \tag{80}$$

$$H^0_{2,0}(\boldsymbol{\nu}) = \frac{\sqrt{5}}{35}\left\{-\left[5\tilde{A}+7\right] A(\nu) + \left[-22\tilde{A}+28\right] B(r_0)\right\}, \tag{81}$$

$$H^0_{2,\pm2}(\boldsymbol{\nu}) = \frac{2\sqrt{5\pi}}{35}\left[-11\tilde{A}+14\right] C(\nu) z_{\pm2}(\boldsymbol{\nu}) \tag{82}$$

$$H^2_{2,2}(\boldsymbol{\nu}) = H^{-2}_{2,-2}(\boldsymbol{\nu}) = \frac{\sqrt{15}}{5}\left[\frac{2\tilde{A}}{7}+1\right] A(\nu), \tag{83}$$

$$H^0_{4,0}(\boldsymbol{\nu}) = \frac{6\tilde{A}}{35}\left[A(\nu) - 4B(\nu)\right], \tag{84}$$

$$H^0_{4,\pm2}(\boldsymbol{\nu}) = -\frac{24\sqrt{\pi}}{35}\tilde{A} C(\nu) z_{\pm2}(\boldsymbol{\nu}), \tag{85}$$

$$H^2_{4,2}(\boldsymbol{\nu}) = H^{-2}_{4,-2}(\boldsymbol{\nu}) = -\frac{3\sqrt{5}}{35}\tilde{A} A(\nu). \tag{86}$$

where

$$A(\nu) = \frac{2}{\pi}\left[\arccos\left(\frac{\nu}{2\nu_o}\right) - \frac{\nu}{2\nu_o}\sqrt{1-\left(\frac{\nu}{2\nu_o}\right)^2}\right]\Pi\left(\frac{\nu}{2\nu_o}\right), \tag{87}$$

$$B(\nu) = \frac{1}{\pi}\left(\frac{\mathrm{NA}}{n_o}\right)^2\left[\arccos\left(\frac{\nu}{2\nu_o}\right) - \left[3-2\left(\frac{\nu}{2\nu_o}\right)^2\right]\frac{\nu}{2\nu_o}\sqrt{1-\left(\frac{\nu}{2\nu_o}\right)^2}\right]\Pi\left(\frac{\nu}{2\nu_o}\right), \tag{88}$$

$$C(\nu) = \frac{1}{\pi}\left(\frac{\mathrm{NA}}{n_o}\right)^2\left[-\frac{4}{3}\frac{\nu}{2\nu_o}\sqrt[3]{1-\left(\frac{\nu}{2\nu_o}\right)^2}\right]\Pi\left(\frac{\nu}{2\nu_o}\right). \tag{89}$$

4.3 Singular value decomposition

We follow the same procedure and plug the transfer function into the frequency-domain eigenvalue problem (Eq. 11) which gives a 3×3 eigenvalue problem

$$\mathsf{K}\mathsf{V}_j = \mu_j\mathsf{V}_j, \tag{90}$$

where the entries of K are given by

$$\mathsf{K}_{00} = \sum_{l,m} H_{l,-2}^m H_{l,-2}^m = \{H_{0,-2}^0\}^2 + \{H_{2,-2}^{-2}\}^2 + \{H_{2,-2}^0\}^2 + \{H_{4,-2}^{-2}\}^2 + \{H_{4,-2}^0\}^2, \tag{91}$$

$$\mathsf{K}_{11} = \sum_{l,m} H_{l,0}^m H_{l,0}^m = \{H_{0,0}^0\}^2 + \{H_{2,0}^0\}^2 + \{H_{4,0}^0\}^2, \tag{92}$$

$$\mathsf{K}_{22} = \sum_{l,m} H_{l,2}^m H_{l,2}^m = \{H_{0,2}^0\}^2 + \{H_{2,2}^2\}^2 + \{H_{2,2}^0\}^2 + \{H_{4,2}^2\}^2 + \{H_{4,2}^0\}^2, \tag{93}$$

$$\mathsf{K}_{01} = \mathsf{K}_{10} = \sum_{l,m} H_{l,-2}^m H_{l,0}^m = H_{0,-2}^0 H_{0,0}^0 + H_{2,-2}^0 H_{2,0}^0 + H_{4,-2}^0 H_{4,0}^0, \tag{94}$$

$$\mathsf{K}_{02} = \mathsf{K}_{20} = \sum_{l,m} H_{l,-2}^m H_{l,2}^m = H_{0,-2}^0 H_{0,2}^0 + H_{2,-2}^0 H_{2,2}^0 + H_{4,-2}^0 H_{4,2}^0, \tag{95}$$

$$\mathsf{K}_{12} = \mathsf{K}_{21} = \sum_{l,m} H_{l,0}^m H_{l,2}^m = H_{0,0}^0 H_{0,2}^0 + H_{2,0}^0 H_{2,2}^0 + H_{4,0}^0 H_{4,2}^0. \tag{96}$$

The eigenvalues and eigenvectors can be computed in a closed form (and I've done this using a symbolic package), but writing the result would fill several pages with notation and provide little insight. Instead we proceed straight to plots of the eigenvalues and eigenvectors shown in Fig. XXX.

References

[1] Herbert H.H. Homeier and E.Otto Steinborn. Some properties of the coupling coefficients of real spherical harmonics and their relation to gaunt coefficients. *Journal of Molecular Structure: THEOCHEM*, 368:31 – 37, 1996. Proceedings of the Second Electronic Computational Chemistry Conference.

[2] http://docs.sympy.org/latest/modules/physics/wigner.html#sympy.physics.wigner.gaunt.

A Calculating products of circular and spherical harmonics

To calculate the kernels of arbitrary microscope designs we need an efficient way to calculate the products of functions that are linear combinations of circular and spherical harmonics. We start by considering the simplest case of multiplying two linear combinations of circular harmonics given by

$$f(\hat{\mathbf{p}}) = \sum_{n=0}^{\infty} c_n z_n(\hat{\mathbf{p}}), \qquad f'(\hat{\mathbf{p}}) = \sum_{n'=0}^{\infty} c'_{n'} z_{n'}(\hat{\mathbf{p}}). \tag{97}$$

The product of these two functions is given by

$$f''(\hat{\mathbf{p}}) = f(\hat{\mathbf{p}})f'(\hat{\mathbf{p}}) = \sum_{n=0}^{\infty}\sum_{n'=0}^{\infty} c_n c'_{n'} z_n(\hat{\mathbf{p}}) z_{n'}(\hat{\mathbf{p}}) = \sum_{n''=0}^{\infty} c''_{n''} z_{n''}(\hat{\mathbf{p}}), \tag{98}$$

and we would like to find a relationship between the input coefficients (c_n $c'_{n'}$) and the output coefficients $c''_{n''}$. To find this relationship we can rewrite the product the circular harmonics as a linear combination of circular harmonics

$$z_n(\hat{\mathbf{p}}) z_{n'}(\hat{\mathbf{p}}) = \sum_{j''=0}^{\infty} P_{n,n',n''} z_{j''}(\hat{\mathbf{p}}) \tag{99}$$

where $P_{n,n'}^{n''}$ are the triple integrals of the circular harmonics

$$P_{n,n',n''} = \int_{\mathbb{S}^1} d\hat{\mathbf{p}}\, z_n(\hat{\mathbf{p}}) z_{n'}(\hat{\mathbf{p}}) z_{n''}(\hat{\mathbf{p}}). \tag{100}$$

Plugging Eq. 99 into Eq. 98 gives

$$\sum_{n=0}^{\infty}\sum_{n'=0}^{\infty} c_n c'_{n'} \left[\sum_{j''=0}^{\infty} P_{n,n'}^{n''} z_{j''}(\hat{\mathbf{p}})\right] = \sum_{n''=0}^{\infty} c''_{n''} z_{n''}(\hat{\mathbf{p}}). \tag{101}$$

Therefore, the coefficients are related by

$$c''_{n''} = \sum_{n=0}^{\infty}\sum_{n'=0}^{\infty} P_{n,n',n''} c_n c'_{n'}. \tag{102}$$

Rewriting this equation in Einstein notation (summation over matching indices is implied, upper indices are "column" indices, lower indices are "row" indices) gives

$$c''^{n''} = P_{n,n'}^{n''} c_n c'_{n'}. \tag{103}$$

We can precompute the triple integrals $P_{n,n',n''}$ using a symbolic package like Sympy.

The discussion above applies to spherical harmonics as well—we only need to replace the triple integral of the circular harmonics $P_{n,n',n''}$ with the triple integral of the spherical harmonics

$$G_{j,j',j''} = \int_{\mathbb{S}^2} d\hat{\mathbf{s}}\, y_j(\hat{\mathbf{s}}) y_{j'}(\hat{\mathbf{s}}) y_{j''}(\hat{\mathbf{s}}). \tag{104}$$

where each of the j indices are a single index over the spherical harmonics. We could compute the triple integrals symbolically, but these integrals can take several minutes. Instead, we can write the integral in terms of the Gaunt coefficients [1] which are products of the Clebsch-Gordan coefficients or Wigner 3-j symbols. The Gaunt coefficients have a closed form expression in terms of j, j', and j'' (usually expressed in terms of l, l', l'', m, m', m'') that is implemented in the Sympy library [2].

To calculate the kernel for general polarized light microscopes we will need to multiply functions in the following form

$$f(\hat{\mathbf{p}}, \hat{\mathbf{s}}) = \sum_{n=0}^{\infty}\sum_{j=0}^{\infty} c_{n,j} z_n(\hat{\mathbf{p}}) y_j(\hat{\mathbf{s}}), \qquad f'(\hat{\mathbf{p}}, \hat{\mathbf{s}}) = \sum_{n'=0}^{\infty}\sum_{j'=0}^{\infty} c'_{n',j'} z_n(\hat{\mathbf{p}}) y_j(\hat{\mathbf{s}}). \tag{105}$$

The product will be in the form

$$f(\hat{\mathbf{p}},\hat{\mathbf{s}})f'(\hat{\mathbf{p}},\hat{\mathbf{s}})=\sum_{n=0}^{\infty}\sum_{j=0}^{\infty}c''_{n'',j''}z_{n''}(\hat{\mathbf{p}})y_{j''}(\hat{\mathbf{s}}), \tag{106}$$

where

$$c''^{n'',j''}=P^{n''}_{n,n'}G^{j''}_{j,j'}c_{n,j}c'_{n',j'}. \tag{107}$$

Equation 107 is the main result of this section. It shows that we can precalculate the triple integrals of the circular and spherical harmonics and use the results to efficiently find the coefficients of the product of two arbitrary kernels. We can think of Eq. 107 as a bilinear map that acts within the vector space of harmonic function coefficients. The bilinear map takes two elements of the vector space and maps them to another element of the vector space by a rank-6 tensor product. A lower dimensional example of a bilinear map is the cross product which takes two vectors in three-dimensional Euclidean space and maps them to another vector by a rank-3 tensor product.