[SANS optimization]
(Chapter 5.4.1 in *Elements*)

SANS Optimization

Here we outline the procedure for optimizing the geometric arrangement of SANS instruments. Such analysis is essential for instrument design. But on a day-to-day or more frequent basis, changes in operating conditions to span different Q-ranges at different resolutions in steady-source instruments need to follow optimization guidelines. Mildner and Carpenter (1984) have carried this out for several cases: small-angle Bragg diffraction and axially symmetric small-angle scattering with constrained *Q,* for a given Q resolution and a fixed total flight path of the diffractometer. We reiterate their analysis for the case of fixed scalar *Q*, in the case of cylindrical component geometry. Subject to given resolution, the counting rate in the detector given previously is to be maximized, and following Mildner and Carpenter, we rewrite combining constant parameters into one overall constant,

$$C_D(Q) = c'\frac{A_1A_2A_3\Delta\lambda}{L_c^2L_D^2} = c\frac{R_1^2R_2^2(R\Delta R)\Delta\lambda}{L_c^2L_D^2}\,, \qquad (5\text{-SO1})$$

in which $Q = \frac{2\pi}{\lambda}\frac{R}{L_D}$. (5-SO2)

<u>Resolution</u>

The variance of the scattering-angle resolution-broadening function is

$$\sigma_\theta^2 = \frac{R_1^2}{4L_c^2} + \frac{R_2^2}{4}\left(\frac{1}{L_c}+\frac{1}{L_D}\right)^2 + \frac{(\Delta R)^2}{12L_D^2}\,, \qquad (5\text{-SO3})$$

where ΔR is the width of a ring of active area on the detector (adapted from Mildner and Carpenter). The overall *Q*-resolution, including the effect of finite wavelength resolution, is

$$\sigma_Q^2 = \left(\frac{2\pi}{\lambda}\right)^2\sigma_\theta^2 + \frac{Q^2}{\lambda^2}\sigma_\lambda^2, \qquad (5\text{-SO4})$$

where the variance of the wavelength distribution is

$$\sigma_\lambda^2 = \frac{(\delta\lambda)^2}{6} + \left(\frac{\frac{h}{m}}{L_{rotor}\omega_{rotor}}\right)^2\frac{(\delta\varphi)^2}{12}\;. \qquad (5\text{-SO5})$$

The velocity selector typically used in steady-source instruments produces a triangular wavelength distribution with FWHM $\delta\lambda$ (see Chapter 9.1.1). Here, $\delta\varphi$ is the FWHM of the angular distribution of neutrons in the beam incident on the rotor, assumed to be rectangular. Experimenters usually select the wavelength by varying the rotor angular velocity ω_{rotor}. Then $\frac{\delta\lambda}{\lambda}$ and $\frac{\sigma_\lambda^2}{\lambda^2}$ are constant, built-in features of the instrument. For simplicity in the following discussion of optimization, we assume that the wavelength distribution is triangular with width

$$\Delta\lambda = \sqrt{6}\sigma_\lambda , \qquad (5\text{-SO6})$$

so that

$$\sigma_Q^2 = k^2\sigma_\theta^2 + \frac{1}{6}k^2\left(\frac{R}{L_D}\right)^2\left(\frac{\Delta\lambda}{\lambda}\right)^2 , \qquad (5\text{-SO7})$$

where k = 2π/λ.

Perhaps it is not usually done, but operators could vary the mean selected wavelength by tilting the rotor axis (but never when the rotor is running), changing the wavelength but not the wavelength resolution if $\delta\varphi$ is fixed (see Chap. 9.1.1 in *Elements*).

Accounting for the penumbra size and the penumbral broadening of the scattered neutrons, the minimum accessible Q is

$$Q_{\min} = 2\mathrm{x}\frac{2\pi}{\lambda}\theta_{\min} = 2\mathrm{x}\frac{2\pi}{\lambda}\frac{r_p(x = L_D)}{L_D} = \frac{4\pi}{\lambda}\left(\frac{R_2}{L_D} + \frac{(R_1 + R_2)}{L_c}\right). \qquad (5\text{-SO8})$$

Optimization process

The optimization process employs the procedure of *Lagrange multipliers*, a method for maximizing or minimizing a function of several variables subject to constraints, that is, *side conditions*, which represent fixed relationships among the variables. Most textbooks on Advanced Calculus discuss the method.

Our problem is to find values of R_1, R_2, L_c, L_D, R, ΔR, and $\Delta\lambda$ (seven variables) that maximize C_D. The resolution σ_Q^2 is fixed. The total instrument length is given: $L_o = L_c + L_D$, in which L_c does not include the lengths of components upstream from the collimator entrance. And $Q = k\frac{R}{L_D}$. These represent three side conditions, that is, constraints. The process requires seven gradient equations, shown later. For convenience we write the side conditions as

$$f = 0,\ g = 0,\ \text{and}\ h = 0. \qquad (5\text{-SO9})$$

The resolution constraint is

$$f = \left[\frac{3R_1^2}{L_c^2} + \frac{3R_2^2}{L'^2} + \frac{(\Delta R)^2}{L_D^2} + 2\frac{R^2}{L_D^2}\left(\frac{\Delta\lambda}{\lambda}\right)^2\right] - \frac{12}{k^2} \qquad (5\text{-SO10})$$

for a triangular wavelength distribution. For a square distribution, the fourth term would be

$$\frac{R^2}{L_D^2}\left(\frac{\Delta\lambda}{\lambda}\right)^2 . \qquad (5\text{-SO11})$$

The length constraint is

$$g = L_c + L_D - L_o = 0, \tag{5-SO12}$$

and the wave vector constraint is

$$h = \frac{R}{L_D} - \frac{Q}{k} = 0. \tag{5-SO13}$$

Here, $\frac{1}{L'} = \frac{1}{L_c} + \frac{1}{L_D}$ and $k = \frac{2\pi}{\lambda}$. The μs are Lagrange multipliers, one for each side condition, introduced to facilitate the optimization. Here, C_D, f, g, and h are functions of the variables and σ_Q^2, L_o, and Q are fixed, given, values. There are seven gradient equations, one for each variable, and three side conditions, with seven variables and three multipliers to be determined. Fortunately, all the functions and derivatives are simple. Following, the gradient equations are on the left and the explicit relationships are on the right:

$$\left\{\begin{aligned}
\frac{\partial C_D}{\partial R_1} &= \mu_1\frac{\partial f}{\partial R_1} + \mu_2\frac{\partial g}{\partial R_1} + \mu_3\frac{\partial h}{\partial R_1},\\
\frac{\partial C_D}{\partial R_2} &= \mu_1\frac{\partial f}{\partial R_2} + \mu_2\frac{\partial g}{\partial R_2} + \mu_3\frac{\partial h}{\partial R_2},\\
\frac{\partial C_D}{\partial L_c} &= \mu_1\frac{\partial f}{\partial L_c} + \mu_2\frac{\partial g}{\partial L_c} + \mu_3\frac{\partial h}{\partial L_c},\\
\frac{\partial C_D}{\partial L_D} &= \mu_1\frac{\partial f}{\partial L_D} + \mu_2\frac{\partial g}{\partial L_D} + \mu_3\frac{\partial h}{\partial L_D},\\
\frac{\partial C_D}{\partial \Delta R} &= \mu_1\frac{\partial f}{\partial \Delta R} + \mu_2\frac{\partial g}{\partial \Delta R} + \mu_3\frac{\partial h}{\partial \Delta R},\\
\frac{\partial C_D}{\partial R} &= \mu_1\frac{\partial f}{\partial R} + \mu_2\frac{\partial g}{\partial R} + \mu_3\frac{\partial h}{\partial R},\\
\frac{\partial C_D}{\partial \Delta\lambda} &= \mu_1\frac{\partial f}{\partial \Delta\lambda} + \mu_2\frac{\partial g}{\partial \Delta\lambda} + \mu_3\frac{\partial h}{\partial \Delta\lambda},
\end{aligned}\right.
\Rightarrow
\left\{\begin{aligned}
&\frac{2C_D}{R_1} = \mu_1\frac{6R_1}{2L_c^2},\\
&\frac{2C_D}{R_2} = \mu_1\frac{6R_2}{L'^2},\\
&\frac{2\,C_D}{L_c} = \mu_1\left(\frac{6R^2}{L_c^3} + \frac{6R_2^2(L_c+L_D)}{L_D L_c^3}\right)\frac{}{L_c^3} - \mu_2,\\
&\frac{2C_D}{L_D} = \mu_1\left(2\frac{(\Delta R)^2}{L_D^3} + 2\frac{R^2}{L_D^3}\left(\frac{\Delta\lambda}{\lambda}\right)^2 + 6\frac{R_2^2}{L_c L_D^3}(L_c+L_D)\right)\\
&\qquad - \mu_2 + \mu_3\frac{R}{L_D^2},\\
&\frac{C_D}{\Delta R} = \mu_1\frac{2\Delta R}{L_D^2},\\
&\frac{C_D}{R} = \mu_1\frac{2R}{L_D^2}\left(\frac{\Delta\lambda}{\lambda}\right)^2 + \mu_3\frac{1}{L_D},\\
&\frac{C_D}{\Delta\lambda} = \mu_1 2\frac{R^2}{L_D^2}\frac{\Delta\lambda}{\lambda^2}.
\end{aligned}\right.
\tag{5-SO14}$$

Eliminating μ_1 from the first two equations yields the relationship

$$\frac{R_1}{R_2} = L_c\left(\frac{1}{L_c} + \frac{1}{L_D}\right) = \frac{L_c + L_D}{L_D}, \text{ that is, } \frac{R_1}{L_c + L_D} = \frac{R_2}{L_D}, \tag{5-SO15}$$

meaning, in geometric interpretation, rays across the extremes of the apertures converge at distance L_D, the location of the detector. This is a universal feature of the double-pinhole collimation arrangements for all cases in Mildner and Carpenter, vector-$\vec{\boldsymbol{Q}}$ (i.e., Bragg scattering) and scalar Q with fixed R or fixed Q.

We leave solving the remaining equations as an exercise to the reader, which may be a little daunting because they are nonlinear in the variables, although they are, after all tractable. The solution yields the optimum conditions:

$$L_c = L_D \text{ and } R_1 = 2R_2 = \sqrt{\frac{2}{3}}\Delta R = \sqrt{\frac{2}{3}}R\left(\frac{\Delta\lambda}{\lambda}\right). \qquad (5\text{-SO16})$$

The optimized angular resolution, in terms of its standard deviation, is then

$$\sigma_\theta = \sqrt{\frac{5}{8}}k\left(\frac{R_1}{L_c}\right) \quad , \qquad (5\text{-SO17})$$

and the minimum accessible Q , for the optimized parameters, is

$$Q_{\min} = 2k\left(\frac{R_1 + R_2}{L_c} + \frac{R_2}{L_D}\right) = 4k\frac{R_1}{L_c}. \qquad (5\text{-SO18})$$

The optimization conditions for vector Q (Bragg scattering) measurements are slightly different and the radial averaging is then inappropriate. The dedicated student may wish to work out the results, which are recorded in Mildner and Carpenter.

Reference

Mildner, D. F. R. and J. M Carpenter (1984) Optimization of the experimental resolution for small angle scattering J. *Appl. Cryst*. **17**, 249-256.