Details of the calculation

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For the fitting step, we minimize the minus log of equation 14.

$$-\log p(\Theta|D) = C^{st} + \log(\sigma^2) + \frac{1}{2}\boldsymbol{\epsilon}^\top \boldsymbol{\Omega}^{-1}\boldsymbol{\epsilon} + \frac{1}{2}\log|\boldsymbol{\Omega}| \quad \text{(A1)}$$

The quasi-Newton optimizer used to minimize the previous equation needs to compute gradients with respect to $\boldsymbol{\Theta}$, and second derivatives are needed as well for the computation of the Hessian. With $E(\mathbf{I}) = -\log p(\mathbf{I}|\mathbf{S}, N, \boldsymbol{\Theta})$, $\mathbf{R} = \boldsymbol{\Omega}^{-1}\boldsymbol{\epsilon}$ and taking into account the symmetry of $\boldsymbol{\Omega}$ and $\boldsymbol{\Omega}^{-1}$

$$\frac{\partial E(\mathbf{I})}{\partial m_k} = -R_k \quad \text{(A2)}$$

$$\frac{\partial E(\mathbf{I})}{\partial \Omega_{kl}} = -\frac{1}{2}R_k R_l + \frac{1}{2}\Omega^{-1}_{lk} \quad \text{(A3)}$$

$$\frac{\partial^2 E(\mathbf{I})}{\partial m_k \partial m_l} = \Omega^{-1}_{kl} \quad \text{(A4)}$$

$$\frac{\partial^2 E(\mathbf{I})}{\partial m_k \partial \Omega_{lm}} = \Omega^{-1}_{lk} R_m \quad \text{(A5)}$$

$$\frac{\partial^2 E(\mathbf{I})}{\partial \Omega_{kl} \partial \Omega_{mn}} = -\frac{1}{2}\Omega^{-1}_{lm}\Omega^{-1}_{nk} + \frac{1}{2}R_k \Omega^{-1}_{lm} R_n + \frac{1}{2}R_n \Omega^{-1}_{km} R_l \quad \text{(A6)}$$

With $\mathbf{L} = \mathbf{\Omega}^{-1}\mathbf{w}(q)$, the derivatives of $\hat{\mathcal{I}}$ are

$$\frac{\partial \hat{\mathcal{I}}(q)}{\partial m(q)} = 1 \tag{A7}$$

$$\frac{\partial \hat{\mathcal{I}}(q)}{\partial m_k} = -L_k \tag{A8}$$

$$\frac{\partial \hat{\mathcal{I}}(q)}{\partial w(q)_k} = R_k \tag{A9}$$

$$\frac{\partial \hat{\mathcal{I}}(q)}{\partial \Omega_{kl}} = -L_k R_l \tag{A10}$$

$$\frac{\partial^2 \hat{\mathcal{I}}(q)}{\partial m(q)^2} = \frac{\partial^2 \hat{\mathcal{I}}(q)}{\partial m(q) \partial m_k} = \frac{\partial^2 \hat{\mathcal{I}}(q)}{\partial m_k \partial m_l} = 0 \tag{A11}$$

$$\frac{\partial^2 \hat{\mathcal{I}}(q)}{\partial m(q) \partial \Omega_{kl}} = 0 \tag{A12}$$

$$\frac{\partial^2 \hat{\mathcal{I}}(q)}{\partial m_k \partial \Omega_{lm}} = L_l \Omega^{-1}_{mk} \tag{A13}$$

$$\frac{\partial^2 \hat{\mathcal{I}}(q)}{\partial \Omega_{kl} \partial \Omega_{mn}} = \Omega^{-1}_{nk}(L_m R_l + L_l R_m) \tag{A14}$$

$$\tag{A15}$$

and the derivatives of $\hat{\sigma_{\mathcal{I}}}^2(q,q)$

$$\frac{\partial \hat{\sigma_{\mathcal{I}}}^2(q,q)}{\partial m(q)} = \frac{\partial \hat{\sigma_{\mathcal{I}}}^2(q,q)}{\partial m_k} = 0 \tag{A16}$$

$$\frac{\partial \hat{\sigma_{\mathcal{I}}}^2(q,q)}{\partial w(q,q)} = 1 \tag{A17}$$

$$\frac{\partial \hat{\sigma_{\mathcal{I}}}^2(q,q)}{\partial w(q)} = -2L_k \tag{A18}$$

$$\frac{\partial \hat{\sigma_{\mathcal{I}}}^2(q,q)}{\partial \Omega_{kl}} = L_k L_l \tag{A19}$$

$$\frac{\partial^2 \hat{\sigma_{\mathcal{I}}}^2(q,q)}{\partial w(q,q) \partial w(q)_k} = \frac{\partial^2 \hat{\sigma_{\mathcal{I}}}^2(q,q)}{\partial w(q,q) \partial \Omega_{kl}} = 0 \tag{A20}$$

$$\frac{\partial^2 \hat{\sigma_{\mathcal{I}}}^2(q,q)}{\partial w(q)_k \partial w(q)_l} = -2\Omega^{-1}_{kl} \tag{A21}$$

$$\frac{\partial^2 \hat{\sigma_{\mathcal{I}}}^2(q,q)}{\partial \Omega_{kl} \partial w(q)_m} = L_k \Omega^{-1}_{lm} + L_l \Omega^{-1}_{mk} \tag{A22}$$

$$\frac{\partial^2 \hat{\sigma_{\mathcal{I}}}^2(q,q)}{\partial \Omega_{kl} \partial \Omega_{mn}} = -L_n(\Omega^{-1}_{km} L_l + \Omega^{-1}_{lm} L_k) \tag{A23}$$

Define $f(q) = m(q) - A$, where $m(q)$ is the mean function (equation 9). $f(q)$ is Hammouda's Generalized Guinier Porod function [1], and is thus independent of A. The derivatives of $f(q)$ are

$$\frac{\partial f(q)}{\partial G} = \frac{f(q)}{G} \tag{A24}$$

$$\frac{\partial f(q)}{\partial R_G} = \begin{cases} -2f(q)\frac{q^2 R_G}{3-s} & q \leq q_1 \\ -f(q)\frac{d-s}{R_G} & q > q_1 \end{cases} \tag{A25}$$

$$\frac{\partial f(q)}{\partial d} = \begin{cases} 0 & q \leq q_1 \\ -f(q)\log\left(\frac{q}{q_1}\right) & q > q_1 \end{cases} \tag{A26}$$

$$\frac{\partial f(q)}{\partial s} = \begin{cases} -f(q)\left(\left(\frac{qR_G}{3-s}\right)^2 + \log q\right) & q \leq q_1 \\ -f(q)\left(\frac{d-s}{2(3-s)} + \log q_1\right) & q > q_1 \end{cases} \tag{A27}$$

$$\tag{A28}$$

The second derivatives of $f(q)$ are

$$\frac{\partial^2 f(q)}{\partial G^2} = 0 \tag{A29}$$

$$\frac{\partial^2 f(q)}{\partial G \partial R_G} = \frac{1}{G}\frac{\partial f(q)}{\partial R_G} \tag{A30}$$

$$\frac{\partial^2 f(q)}{\partial G \partial d} = \frac{1}{G}\frac{\partial f(q)}{\partial d} \tag{A31}$$

$$\frac{\partial^2 f(q)}{\partial G \partial s} = \frac{1}{G}\frac{\partial f(q)}{\partial s} \tag{A32}$$

$$\frac{\partial^2 f(q)}{\partial R_G^2} = \begin{cases} f(q)\frac{2q^2}{3-s}\left(\frac{2q^2R_G^2}{3-s} - 1\right) & q \leq q_1 \\ f(q)\frac{d-s}{R_G^2}(d-s+1) & q > q_1 \end{cases} \tag{A33}$$

$$\frac{\partial^2 f(q)}{\partial R_G \partial d} = \begin{cases} 0 & q \leq q_1 \\ -\frac{f(q)}{R_G} - \frac{d-s}{R_G}\frac{\partial f(q)}{\partial d} & q > q_1 \end{cases} \tag{A34}$$

$$\frac{\partial^2 f(q)}{\partial R_G \partial s} = \begin{cases} -2\frac{q^2 R_G}{3-s}\left(\frac{\partial f(q)}{\partial s} + \frac{f(q)}{3-s}\right) & q \leq q_1 \\ \frac{1}{R_G}\left(f(q) - (d-s)\frac{\partial f(q)}{\partial s}\right) & q > q_1 \end{cases} \tag{A35}$$

$$\frac{\partial^2 f(q)}{\partial d^2} = \begin{cases} 0 & q \leq q_1 \\ f(q)\left(\log^2\left(\frac{q}{q_1}\right) + \frac{1}{2(d-s)}\right) & q > q_1 \end{cases} \tag{A36}$$

$$\frac{\partial^2 f(q)}{\partial d \partial s} = \begin{cases} 0 & q \leq q_1 \\ -\log\left(\frac{q}{q_1}\right)\frac{\partial f(q)}{\partial s} - \left(\frac{1}{3-s} + \frac{1}{d-s}\right)\frac{f(q)}{2} & \end{cases} \tag{A37}$$

$$\frac{\partial^2 f(q)}{\partial s^2} = \begin{cases} f(q)\left(\left[\left(\frac{qR_G}{3-s}\right)^2 + \log q\right]^2 - 2\frac{(qR_G)^2}{(3-s)^3}\right) \\ f(q)\left(\left[\frac{d-s}{2(3-s)} + \log q_1\right]^2 + \frac{1}{2}\left[\frac{6-s-d}{(3-s)^2} + \frac{1}{d-s}\right]\right) \end{cases} \tag{A38}$$

The derivatives of the covariance function (equation 5) are

$$\frac{\partial w(q,q')}{\partial \tau} = \frac{2}{\tau} w(q,q') \tag{A39}$$

$$\frac{\partial^2 w(q,q')}{\partial \tau^2} = \frac{2}{\tau^2} w(q,q') \tag{A40}$$

$$\frac{\partial w(q,q')}{\partial \lambda} = \frac{1}{\lambda}\left(\frac{q-q'}{\lambda}\right)^2 w(q,q') \tag{A41}$$

$$\frac{\partial^2 w(q,q')}{\partial \lambda^2} = w(q,q') \times \frac{1}{\lambda^2}\left(\frac{q-q'}{\lambda}\right)^2 \left[\left(\frac{q-q'}{\lambda}\right)^2 - \frac{3}{2}\right] \tag{A42}$$

$$\frac{\partial^2 w(q,q')}{\partial \lambda \partial \tau} = \frac{2}{\tau}\frac{\partial w(q,q')}{\partial \lambda} \tag{A43}$$

The derivatives and the Hessian are calculated by following the chain rule. For example

$$\frac{\partial E(\mathbf{I})}{\partial \Theta_i} = \sum_k \frac{\partial E(\mathbf{I})}{\partial m_k}\frac{\partial m_k}{\partial \Theta_i} + \sum_{k,l}\frac{\partial E(\mathbf{I})}{\partial \Omega_{kl}}\frac{\partial \Omega_{kl}}{\partial \Theta_i} \tag{A44}$$

$$\begin{aligned}\frac{\partial^2 E(\mathbf{I})}{\partial \Theta_i \partial \Theta_j} &= \sum_{k,l}\frac{\partial^2 E(\mathbf{I})}{\partial m_k \partial m_l}\frac{\partial m_k}{\partial \Theta_i}\frac{\partial m_l}{\partial \Theta_j} + \sum_{k,l,m,n}\frac{\partial^2 E(\mathbf{I})}{\partial \Omega_{kl}\partial \Omega_{mn}}\frac{\partial \Omega_{kl}}{\partial \Theta_i}\frac{\partial \Omega_{mn}}{\partial \Theta_j} \\ &+ \sum_{k,l,m}\frac{\partial^2 E(\mathbf{I})}{\partial m_k \partial \Omega_{lm}}\left(\frac{\partial m_k}{\partial \Theta_j}\frac{\partial \Omega_{lm}}{\partial \Theta_i} + \frac{\partial m_k}{\partial \Theta_i}\frac{\partial \Omega_{lm}}{\partial \Theta_j}\right) \\ &+ \sum_k \frac{\partial E(\mathbf{I})}{\partial m_k}\frac{\partial^2 m_k}{\partial \Theta_i \partial \Theta_j} + \sum_{k,l}\frac{\partial E(\mathbf{I})}{\partial \Omega_{kl}}\frac{\partial^2 \Omega_{kl}}{\partial \Theta_i \partial \Theta_j}\end{aligned} \tag{A45}$$

References

[1] B. Hammouda. A new Guinier-Porod model. *J Appl Cryst*, 43:716–719, May 2010.