Quadratic background correction within RMC

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If we want to compute the coefficients of a quadratic background within RMC we would calculate χ^2 from the following expression:

$$\chi^2 = \sum_{i=1}^{N} \sum_{p=1}^{N_i} \frac{\left(F_i(Q_{ip}) - \alpha_i S(Q_{ip}) - \sum_{j=0}^{2} a_{ij} Q_{ip}^j \right)^2}{\sigma_i^2(Q_{ip})}, \tag{1}$$

where we sum over the N sets of experimental results and the points of Q_{ip} (modules of each scattering vector). F_i is the scattering function from the i th experiment and S is the same function calculated from the configuration. α_i denotes the normalisation, and a_{ij} denotes the j-th order coefficient of the Q dependent polynomial background.

In the next two section; I am describing a computation method to calculate these coefficients and (1).

1 Calculation of the coefficients

Since coefficients of one experiment are independent from another one's and in the actual version of RMC it is not possible to define Q-dependent standard deviation[1], we consider the simplified version of (1) as follows:

$$\begin{aligned} \chi^2 &= \sum_{i=1}^{N} \frac{\chi_i'^2}{\sigma_i^2} \\ \chi'^2 &= \sum_{p=1}^{N_i} \left(F_p - \alpha S_p - \sum_{j=0}^{2} a_j Q_p^j \right)^2 \end{aligned} \tag{2}$$

Let's look for the values of coefficients for which this expression will be minimal, we will able to get them if we choose them so that the first derivatives of this expression by each coefficient will be equal to zero:

$$\begin{aligned} 0 &= \frac{\partial \chi'^2}{\partial a_k} = \sum_{p=1}^{N_i} \left(\alpha S_p Q_p^k + \sum_{j=0}^{2} a_j Q_p^{k+j} - F_p Q_p^k \right) \cdot 2 \\ 0 &= \frac{\partial \chi'^2}{\partial \alpha} = \sum_{p=1}^{N_i} \left(\alpha S_p^2 + \sum_{j=0}^{2} a_j Q_p^j S_p - F_p S_p \right) \cdot 2 \end{aligned} \tag{3}$$

These equations are linear equations which can be solved by Gauss elimination[2]. The general form of the matrix equation can by written in this form, where the capitals are the matrix elements:

$$(\ A\ B\ C\ D\ E\ ) \ \Rightarrow\ A \cdot a_2 + B \cdot a_1 + C \cdot a_0 + D \cdot \alpha = E \tag{4}$$

In the next part, I am discussing the cases of fixing and/or fitting these coefficients.

[1] In this case it is taken into account a w_p weight factor in (1).
[2] The calculation of the coefficients of more than two order polynomial will be faster if you use an iteration method.

1.1 Trivial case – all coefficients to be fixed

This is the simplest case – the coefficients are:

$$\alpha = 1.0\ ,\ a_0 = 0.0\ ,\ a_1 = 0.0\ ,\ a_2 = 0.0 \tag{5}$$

1.2 Calculation of one coefficient

This occurs in four cases:

$$\begin{aligned} \alpha : &\qquad \left(\begin{array}{cc} \sum\limits_p S_p^2 & \sum\limits_p F_p S_p \end{array} \right) \\ a_m : &\qquad \left(\begin{array}{cc} \sum\limits_p Q_p^{2m} & \sum\limits_p F_p Q_p^m - \sum\limits_p S_p Q_p^m \end{array} \right), \end{aligned} \tag{6}$$

So we can obtain:

$$\begin{aligned} \alpha &= \frac{\sum\limits_p F_p S_p}{\sum\limits_p S_p^2},\ a_0 = \frac{\sum\limits_p F_p - \sum\limits_p S_p}{N_i}, \\ a_1 &= \frac{\sum\limits_p F_p Q_p - \sum\limits_p S_p Q_p}{\sum\limits_p Q_p^2},\ a_2 = \frac{\sum\limits_p F_p Q_p^2 - \sum\limits_p S_p Q_p^2}{\sum\limits_p Q_p^4} \end{aligned} \tag{7}$$

1.3 Calculation of two coefficients simultaneously

These calculation occur in six cases. Equations could be written in the following form ($m > l$):

$$\begin{aligned} a_m,\ \alpha : &\quad \left(\begin{array}{ccc} \sum\limits_p Q_p^{2m} & \sum\limits_p S_p Q_p^m & \sum\limits_p F_p Q_p^m \\ \sum\limits_p S_p Q_p^m & \sum\limits_p S_p^2 & \sum\limits_p F_p S_p \end{array} \right) \\ a_m,\ a_l : &\quad \left(\begin{array}{ccc} \sum\limits_p Q_p^{2m} & \sum\limits_p Q_p^{m+l} & \sum\limits_p F_p Q_p^m - \sum\limits_p S_p Q_p^m \\ \sum\limits_p Q_p^{m+l} & \sum\limits_p Q^{2l} & \sum\limits_p F_p Q_p^l - \sum\limits_p S_p Q_p^l \end{array} \right) \end{aligned} \tag{8}$$

The determinant of the generalised form of these systems of equations is:

$$\left| \begin{array}{ccc} A & B & C \\ B & D & E \end{array} \right| \tag{9}$$

Solving this equation (by Cramer-method), we can get:

$$\begin{aligned} y &= \frac{AE - BC}{AD - B^2} \\ x &= \frac{C - By}{A} \end{aligned} \tag{10}$$

Substituting the terms from table 1, solutions are found.

1.4 Calculations of three coefficients simultaneously

If we fit three coefficients at the same time, we will solve the next systems of equations ($m > l$):

$$\begin{aligned} a_m,\ a_l,\ \alpha : &\left(\begin{array}{cccc} \sum\limits_p Q_p^{2m} & \sum\limits_p Q_p^{m+l} & \sum\limits_p S_p Q_p^m & \sum\limits_p F_p Q_p^m \\ \sum\limits_p Q_p^{m+l} & \sum\limits_p Q_p^{2m} & \sum\limits_p S_p Q_p^l & \sum\limits_p F_p Q_p^l \\ \sum\limits_p S_p Q_p^m & \sum\limits_p S_p Q_p^l & \sum\limits_p S_p^2 & \sum\limits_p F_p S_p \end{array} \right) \\ a_2,\ a_1,\ a_0 : &\left(\begin{array}{cccc} \sum\limits_p Q_p^4 & \sum\limits_p Q_p^3 & \sum\limits_p Q_p^2 & \sum\limits_p F_p Q_p^2 - \sum\limits_p S_p Q_p^2 \\ \sum\limits_p Q_p^3 & \sum\limits_p Q_p^2 & \sum\limits_p Q_p & \sum\limits_p F_p Q_p - \sum\limits_p S_p Q_p \\ \sum\limits_p Q_p^2 & \sum\limits_p Q_p & N_i & \sum\limits_p F_p - \sum\limits_p S_p \end{array} \right) \end{aligned} \tag{11}$$

Table 1: Substitution values of the elements of the general determinant to eq. (10) in the case of two coefficient fitting.

x	a_2	a_2	a_2	a_1	a_1	a_0
y	a_1	a_0	α	a_0	α	α
A	$\sum_p Q_p^4$	$\sum_p Q_p^4$	$\sum_p Q_p^4$	$\sum_p Q_p^2$	$\sum_p Q_p^2$	N_i
B	$\sum_p Q_p^3$	$\sum_p Q_p^2$	$\sum_p S_p Q_p^2$	$\sum_p Q_p$	$\sum_p S_p Q_p$	$\sum_p S_p$
C	$\sum_p F_p Q_p^2 - \sum_p S Q_p^2$	$\sum_p F_p Q_p^2 - \sum_p S_p Q_p^2$	$\sum_p F_p Q_p^2$	$\sum_p F_p Q_p - \sum_p S_p Q_p$	$\sum_p F_p Q_p$	$\sum_p F_p$
D	$\sum_p Q_p^2$	N_i	$\sum_p S_p^2$	N_i	$\sum_p S_p^2$	$\sum_p S_p^2$
E	$\sum_p F_p Q_p - \sum_p S Q_p$	$\sum_p F_p - \sum_p S_p$	$\sum_p F_p S_p$	$\sum_p F_p - \sum_p S_p$	$\sum_p F_p S_p$	$\sum_p F_p S_p$

The determinant of the generalised form of this system of equations is:

$$\begin{pmatrix} a & b & c & d \\ b & e & f & g \\ c & f & h & i \end{pmatrix} \tag{12}$$

We substitute:

$$\begin{aligned} A &= ae - b^2 \\ B &= af - bc \\ C &= ag - bd \\ D &= ah - c^2 \\ E &= ai - cd \end{aligned} \tag{13}$$

Performing the first steps of the Gauss elimination in eq. (12) we can get the matrix in the following form:

$$\begin{pmatrix} a & b & c & d \\ 0 & \frac{A}{ab} & \frac{B}{ab} & \frac{C}{ab} \\ 0 & \frac{B}{ac} & \frac{D}{ac} & \frac{E}{ac} \end{pmatrix} \tag{14}$$

Because of the multiplication of one row of the matrix by the same number doesn't change the value of coefficients, we can multiply the second row by ab and the third one by ac. If we are looking at this result, we could observe that this is the same as eq. (9). So we could get the values of coefficients using eq. (10) and :

$$\begin{aligned} Z &= y \\ Y &= x \\ X &= \frac{d - cZ - bY}{a} \end{aligned} \tag{15}$$

Finally, substituting the terms from table 2, we are obtaining the solutions.

1.5 Fitting the coefficients of the second order polynomial and the renormalisation coefficient

First, we write the matrix of the systems of equations, after that it will be originated in the solution of (12) using the Gauss elimination procedure.

The matrix is:

$$\begin{pmatrix} \sum_p Q_p^4 & \sum_p Q_p^3 & \sum_p Q_p^2 & \sum_p S_p Q_p^2 & \sum_p F_p Q_p^2 \\ \sum_p Q_p^3 & \sum_p Q_p^2 & \sum_p Q_p & \sum_p S_p Q_p & \sum_p F_p Q_p \\ \sum_p Q_p^2 & \sum_p Q_p & N_i & \sum_p S_p & \sum_p F_p \\ \sum_p S_p Q_p^2 & \sum_p S_p Q_p & \sum_p S_p & \sum_p S_p^2 & \sum_p F_p S_p \end{pmatrix} \tag{16}$$

Table 2: Substitution values of the elements of the general determinant to eq. (12) in the case of three coefficient fitting.

X	a_2	a_2	a_2	a_1
Y	a_1	a_1	a_0	a_0
Z	a_0	α	α	α
a	$\sum_p Q_p^4$	$\sum_p Q_p^4$	$\sum_p Q_p^4$	$\sum_p Q_p^2$
b	$\sum_p Q_p^3$	$\sum_p Q_p^3$	$\sum_p Q_p^2$	$\sum_p Q_p$
c	$\sum_p Q_p^2$	$\sum_p S_p Q_p^2$	$\sum_p S_p Q_p^2$	$\sum_p S_p Q_p$
d	$\sum_p F_p Q_p^2 - \sum_p S_p Q_p^2$	$\sum_p F_p Q_p^2$	$\sum_p F_p Q_p^2$	$\sum_p F_p Q_p$
e	$\sum_p Q_p^2$	$\sum_p Q_p^2$	N_i	N_i
f	$\sum_p Q_p$	$\sum_p S_p Q_p$	$\sum_p S_p$	$\sum_p S_p$
g	$\sum_p F_p Q_p - \sum_p S_p Q_p$	$\sum_p F_p Q_p$	$\sum_p F_p$	$\sum_p F_p$
h	N_i	$\sum_p S_p^2$	$\sum_p S_p^2$	$\sum_p S_p^2$
i	$\sum_p F_p - \sum_p S_p$	$\sum_p F_p S_p$	$\sum_p F_p S_p$	$\sum_p F_p S_p$

We would like to trace it back to (12), so we ought to reduce matrix (16) to the following form by Gauss elimination:

$$\begin{pmatrix} \sum_p Q_p^4 & \sum_p Q_p^3 & \sum_p Q_p^2 & \sum_p S_p Q_p^2 & \sum_p F_p Q_p^2 \\ 0 & \frac{a}{\sum_p Q_p^4 \sum_p Q_p^3} & \frac{b}{\sum_p Q_p^4 \sum_p Q_p^3} & \frac{c}{\sum_p Q_p^4 \sum_p Q_p^3} & \frac{d}{\sum_p Q_p^4 \sum_p Q_p^3} \\ 0 & \frac{b}{\sum_p Q_p^4 \sum_p Q_p^2} & \frac{e}{\sum_p Q_p^4 \sum_p Q_p^2} & \frac{f}{\sum_p Q_p^4 \sum_p Q_p^2} & \frac{g}{\sum_p Q_p^4 \sum_p Q_p^2} \\ 0 & \frac{c}{\sum_p Q_p^4 \sum_p S_p Q_p^2} & \frac{f}{\sum_p Q_p^4 \sum_p S_p Q_p^2} & \frac{h}{\sum_p Q_p^4 \sum_p S_p Q_p^2} & \frac{i}{\sum_p Q_p^4 \sum_p S_p Q_p^2} \end{pmatrix} \tag{17}$$

It is possible, of course, so that we should use the next substitution:

$$\begin{aligned} a &= \sum_p Q_p^4 \sum Q_p^2 - \left(\sum_p Q_p^3\right)^2 \\ b &= \sum_p Q_p^4 \sum Q_p - \sum_p Q_p^3 \sum_p Q_p^2 \\ c &= \sum_p Q_p^4 \sum S_p Q_p - \sum_p Q_p^3 \sum_p S_p Q_p^2 \\ d &= \sum_p Q_p^4 \sum F_p Q_p - \sum_p Q_p^3 \sum_p F_p Q_p^2 \\ e &= \sum_p Q_p^4 N_i - \left(\sum_p Q_p^2\right)^2 \\ f &= \sum_p Q_p^4 \sum S_p - \sum_p Q_p^2 \sum_p S_p Q_p^2 \\ g &= \sum_p Q_p^4 \sum F_p - \sum_p Q_p^2 \sum_p F_p Q_p^2 \\ h &= \sum_p Q_p^4 \sum S_p^2 - \left(\sum_p S_p Q_p^2\right)^2 \\ i &= \sum_p Q_p^4 \sum F_p S_p - \sum_p F_p Q_p^2 \sum_p S_p Q_p^2 \end{aligned} \tag{18}$$

Finally, the substitution below is needed to be taken into account for obtaining the coefficients:

$$\begin{aligned}
\alpha &= Z \\
a_0 &= Y \\
a_1 &= X \\
a_2 &= \frac{\sum\limits_p F_p Q_p^2 - \alpha \sum\limits_p S_p Q_p^2 - a_0 \sum\limits_p Q_p^2 - a_1 \sum\limits_p Q_p^3}{\sum\limits_p Q_p^4}
\end{aligned} \tag{19}$$

2 Calculation of χ^2

Knowing the values of the coefficients, the calculation of χ^2 is an easy task, just we should extract its form in the case when the uncertainty is Q-independent[3]:

$$\begin{aligned}
\chi^2 = \sum_{i=1}^{N} \frac{1}{\sigma_i^2} \Bigg\{ & \sum_p F_{ip}^2 + \alpha^2 \sum_p S_{ip}^2 + a_0^2 N_i + \left(a_1^2 + 2a_0 a_2\right) \sum_p Q_{ip}^2 + a_2^2 \sum_p Q_{ip}^4 + \\
& + 2 \left[\alpha \left(a_0 \sum_p S_{ip} + a_1 \sum_p S_{ip} Q_{ip} + a_2 \sum_p S_{ip} Q_{ip}^2 - \sum_p F_{ip} S_{ip} \right) + \right. \\
& \left. + a_0 \left(a_1 \sum_p Q_{ip} - \sum_p F_{ip} \right) + a_1 \left(a_2 \sum_p Q_{ip}^3 - \sum_p F_{ip} Q_{ip} \right) - a_2 \sum_p F_{ip} Q_{ip}^2 \right] \Bigg\}
\end{aligned} \tag{20}$$

[3]If not, each term should be multiplied byw_{ip}^2 so that $\sum\limits_{p=1}^{Ni} w_{ip}^2 = N_i$ will be. In this case we should substitute the mean uncertainty $\bar{\sigma_i^2}$ instead of σ_i^2