The SQUAW Fitting Procedure

FOREWORD:

The program SQUAW was legendary in its day for providing a versatile and rigorous treatment of kinematic fitting for particle physics events. The techniques employed by SQUAW are still useful for a wide variety of particle physics problems. What follows is a transcription of parts of the SQUAW manual that provide the details on the fitting procedure. The original source of this material is an old printed copy of the Group A Programming Note No. P-126 dated July 1968, with O.I. Dahl, T.B. Day, T. Solmitz, and N.L. Gould listed as authors. The material was transcribed to TeX by Winnie Isom of Brown University. Please send any corrections to Richard Partridge at richp@slac.stanford.edu.

NOTATION:

We first define several quantities that are used in the fitting procedure. In deriving the basic equations we treat the variables and constraints in a general fashion an therefore do not need to specify their particular form. Throughout this section matrix notation is used.

m = Measured values of well measured variables.

m^* = Measured values of badly measured variables.

G = Inverse square error matrix for m:

$$\left(G_{ij}^{-1} = \overline{\delta m_i \delta \widetilde{m}_j}\right).$$

G^* =Inverse square error matrix for m^*:

$$\left(G_{ij}^{*-1} = \overline{\delta m_i^* \delta \widetilde{m}_j^*}\right).$$

x =Fitted values of well-measured variables.

x^* =Fitted values of badly-measured variables.

$\bar{x}$ =Approximate values of x.

$\bar{x}^*$ =Approximate values of x^*.

f =The vector of constraints.

B =Constraint derivative matrix for well-measured variables:

$$\Big(B_{i\lambda} = \frac{\partial f_\lambda}{\partial x_i}\Big).$$

B^* =Constraint derivative matrix for badly-measured variables:

$$\Big(B^*_{j\lambda} = \frac{\partial f_\lambda}{\partial x_{j*}}\Big).$$

α =Vector of LaGrange multipliers.

E =Error matrix for x:

$$\big(E_{ij} = \overline{\delta x_i \delta \widetilde{x}_j}\big).$$

E^* =Error matrix for x^*:

$$\big(E^*_{ij} = \overline{\delta x^*_i \delta \widetilde{x}^*_j}\big)$$

E^c =Correlation matrix for x and x^*:

$$\big(E^c_{ij} = \overline{\delta x_i \delta \widetilde{x} j^*}\big).$$

It is convenient to work in terms of corrections to the measured values rather than the fitted values themselves. Thus we define

$$c = x - m \qquad 1a)$$

$$c^* = x^* - m^* \tag{1b}$$

$$\bar{c} = \bar{x} - m \tag{1c}$$

$$\bar{c^*} = \bar{x^*} - m^* \tag{1d}$$

Obviously,

$$\frac{\partial f_\lambda}{\partial c_i} = \frac{\partial f_\lambda}{\partial x_i} = B_{i\lambda} \tag{2a}$$

and

$$\frac{\partial f_\lambda}{\partial c_j^*} = \frac{\partial f_\lambda}{\partial x_j^*} = B_{j\lambda}^* \tag{2b}$$

INPUT DATA

We are given as input data values of m, m^*, G^{-1}, and G^*. Here we assume that we can separate these variables into two groups: those which are well measured and those which are poorly measured. This separation is not completely arbitrary; it is controlled by the nature of the measurements. First we must assume that

$$\overline{\delta m \delta \widetilde{m}^*} = 0.$$

That is, we may split up the variables into two groups. Also, for the well measured quantities, G^{-1} must be well defined, although G need not be; whereas for the badly measured quantities G^* must be well defined although G^{*-1} may not be. Thus, well measured variables may have zero error (or be 100% correlated) but they may not be unknown. On the other hand, badly measured variables may be unknown (and hence have a zero weight), but may not have zero error. ("Fixed variables" are considered to be constants and are not treated as variables.) We shall, at times, however, use the quantities G and G^{*-1} in definitions and in derivations, although they will never appear in any equations that must be used explicitly. In these cases they are to be understood in the sense of a limit. To define G^{*-1}, we treat missing quantities as having error δ and let δ approach infinity.

BASIC PROCEDURE

Now we may proceed to find the fitted variables x and x^*. We wish to minimize the quantity

$$\chi^2 = (x^* \widetilde{-} m^*) G^* (x^* - m^*) + (x \widetilde{-} m) G (x - m) \tag{3}$$

subject to the condition

$$f(x, x^*) = 0. \tag{4}$$

Following the usual procedure, we introduce LaGrangian multiplier, α, and define

$$M = 2\widetilde{f}\alpha + \chi^2 = 2\widetilde{f}\alpha + \widetilde{c}^* G^* c^* + \widetilde{c} G c \tag{5}$$

We now wish to minimize M with respect to α, x^*, and x. Thus we have,

$$0 = \frac{1}{2}\frac{\partial M}{\partial \alpha} = f(x^*, x) \tag{6a}$$
$$0 = \frac{1}{2}\frac{\partial M}{\partial x^*} = B^*\alpha + G^* c^* \tag{6b}$$
$$0 = \frac{1}{2}\frac{\partial M}{\partial x} = B\alpha + Gc \tag{6c}$$

To find the values of x^* and x, we must now solve equations 6. In general, since the constraints f are non-linear, this is a very difficult problem. We need to know $f(x^*, x)$, $B(x^*, x)$ and $B^*(x^*, x)$. However, we may simplify the problem by assuming that the constraints are reasonably linear. We pick a trial solution $(\bar{x^*}, \bar{x})$ and expand equation 6a to the first order about this point:

$$\begin{aligned} 0 =& f(x^*, x) = f(\bar{x^*}, \bar{x}) + \widetilde{B}^*[x^* - \bar{x^*}] + \widetilde{B}[x - \bar{x}] \\ =& f + \widetilde{B^*}(c^* - \bar{c^*}) + \widetilde{B}(c - \bar{c}) \end{aligned}$$

or

$$\widetilde{B^*} c^* + \widetilde{B} c = r \tag{7}$$

where

$$r = \widetilde{B^*}\bar{c^*} + \widetilde{B}\bar{c} - f. \tag{8}$$

All derivatives are evaluated at the point $(\bar{x^*}, \bar{x})$. Now the problem is readily solvable. First solve equation 6c for c, getting

$$c = -G^{-1} B\alpha. \tag{9}$$

Upon substituting equation 9 in equation 7, we find

$$-H\alpha + \widetilde{B^*}c^* = r \tag{10}$$

where

$$H = \widetilde{B}G^{-1}B. \tag{11}$$

Now we may combine equation 10 and 6b to get,

$$\begin{pmatrix} -H & \widetilde{B^*} \\ B^* & G^* \end{pmatrix} \begin{pmatrix} \alpha \\ c^* \end{pmatrix} = \begin{pmatrix} r \\ 0 \end{pmatrix} \tag{12}$$

(Note: These are stored in the matrices labeled HH, ALPHA and RR respectively.)

and find α and c^* by solving equation 12. Then we calculate c by using equation 9. We must be slightly careful here. Since both H and G^* may separately be singular, we must solve equation 12 as a whole and may not break it up into equation 10 and 6b and solve first by eliminating either α or c^*.

However, since we have not solved the problem exactly but only in a linear approximation, we must check the new values of x^* and x to see if they satisfy the original equation (6). If they do not we may use these values as new estimates $(\bar{x^*}, \bar{x})$ and repeat the procedure.

Calculation of χ^2

We also wish to calculate the value of χ^2. Define

$$\begin{pmatrix} -H & \widetilde{B^*} \\ B^* & G^* \end{pmatrix}^{-1} = \begin{pmatrix} W & \widetilde{V} \\ V & U \end{pmatrix} \tag{13}$$

Then from equation 9, 12, and 13 we have

$$c^* = Vr \tag{14a}$$

$$\alpha = Wr \tag{14b}$$

$$c = -[G^{-1}B]Wr \tag{14c}$$

If we expand equation 13 we get,

$$\widetilde{B^*}V - HW = 1 \tag{15a}$$

$$\widetilde{B^*}U - H\widetilde{V} = 0 \tag{15b}$$

$$G^*V + B^*W = 0 \tag{15c}$$

$$G^*U + B^*\widetilde{V} = 1 \tag{15d}$$

Now from equations 3, 14, and 15 we get:

$$\begin{aligned}
\chi^2 =& \widetilde{c^*}G^*c^* + \widetilde{c}Gc \\
=& \widetilde{r}\widetilde{V}G^*Vr + \widetilde{r}W\widetilde{B}G^{-1}GG^{-1}BWr \\
=& \widetilde{r}\big\{\widetilde{V}G^*V + WHW\big\}r \\
=& \widetilde{r}\big\{[-W\widetilde{B^*}]V + W[\widetilde{B^*}V - 1]\big\}r = -\widetilde{r}Wr = -\widetilde{\alpha}r
\end{aligned}$$

or

$$\chi^2 = -\widetilde{\alpha}r \tag{16}$$

Calculation of Errors

When we have a solution we also wish to calculate the fitted error matrices E, E^c, and E^*. We have,

$$\frac{\partial r}{\partial m} = -B; \qquad \frac{\partial r}{\partial m^*} = -B^* \tag{17}$$

Thus, we get from equation 14, 15, and 17:

$$\frac{\partial x}{\partial m} = \frac{\partial(m+c)}{\partial m} = 1 + BW[\widetilde{B}G^{-1}] \tag{18a}$$

$$\frac{\partial x}{\partial m^*} = \frac{\partial(m+c)}{\partial m^*} = B^*W\widetilde{B}G^{-1} = -G^*V[\widetilde{B}G^{-1}] \tag{18b}$$

$$\frac{\partial x^*}{\partial m} = \frac{\partial (m^* + c^*)}{\partial m} = -B\widetilde{V} \tag{18c}$$

$$\frac{\partial x^*}{\partial m^*} = \frac{\partial (m^* + c^*)}{\partial m^*} = 1 - B^*\widetilde{V} = G^*U \tag{18d}$$

Now, from equations 15 and 18,

$$\begin{aligned} E =& \overline{\delta x \delta \widetilde{x}} = \frac{\widetilde{\partial} x}{\partial m} G^{-1} \frac{\partial x}{\partial m} + \frac{\partial \widetilde{x}}{\partial m^*} G^{*-1} \frac{\partial x}{\partial m^*} \\ =& [1 + G^{-1} B W \widetilde{B}] G^{-1} [1 + B W \widetilde{B} G^{-1}] \\ =& [G^{-1} B \widetilde{V} G^*] G^{*-1} [G^* V \widetilde{B} G^{-1}] \\ =& G^{-1} + G^{-1} B [2W + WHW + \widetilde{V} G^* V] \widetilde{B} G^{-1}. \end{aligned}$$

But,

$$2W + WHW + \widetilde{V} G^* V = 2W + W[\widetilde{B}^* V - 1] + [-W\widetilde{B}^*]V = W$$

and hence,

$$E = G^{-1} + [G^{-1}B] W [\widetilde{B} G^{-1}]. \tag{19a}$$

$$\begin{aligned} E^c =& \overline{\delta x \delta \widetilde{x}^*} = \frac{\widetilde{\partial} x}{\partial m} G^{-1} \frac{\partial x^*}{\partial m} + \frac{\partial \widetilde{x}}{\partial m^*} G^{*-1} \frac{\partial x^*}{\partial m^*} \\ =& [1 + G^{-1} B W \widetilde{B}] G^{-1} [-B\widetilde{V}] + [-G^{-1} B \widetilde{V} G^*] G^{*-1} [G^* U] \\ =& - G^{-1} B [\widetilde{V} + WH\widetilde{V} + \widetilde{V} G^* U] \end{aligned}$$

But

$$\widetilde{V} + WH\widetilde{V} + \widetilde{V} G^* U = \widetilde{V} + [\widetilde{V} B^* - 1]\widetilde{V} + \widetilde{V}[1 - B^*\widetilde{V}] = \widetilde{V}$$

and

$$E^c = -[G^{-1}B]\widetilde{V}. \tag{19b}$$

$$\begin{aligned} E^* =& \overline{\delta x^* \delta \widetilde{x}^*} = \frac{\partial \widetilde{x}^*}{\partial m} G^{-1} \frac{\partial x^*}{\partial m} + \frac{\partial \widetilde{x}^*}{\partial m^*} G^{*-1} \frac{\partial x^*}{\partial m^*} \\ =& [-V\widetilde{B}] G^{-1} [-B\widetilde{V}] + [UG^*] G^{*^{-1}} [G^* U] \\ =& VH\widetilde{V} + UG^*U = V[\widetilde{B}^* U] + [1 - V\widetilde{B}^*]U = U \end{aligned}$$

or

$$E^* = U \tag{19c}$$

Pull Quantities

We may also calculate some useful test functions. Define the pull quantities as

$$\xi_i = \frac{c_i}{\sqrt{\overline{c_i^2}}} \tag{20}$$

Obviously, if our input measurements and errors are correctly assigned and our various assumptions hold, ξ_i is a quantity which should have a mean of zero and a width of 1. We may use these pull quantities to calibrate our error assignments and to check for some type of biases in the data.

To form the pull quantities we must calculate the r.m.s. correction for each variable. (For the moment let us not distinguish between well measured and badly measured variables.) Since on an individual measurement we have

$$\delta x = \delta m + c$$

we get

$$\overline{\delta m \delta \widetilde{m}} = \overline{\delta x \delta \widetilde{x}} + \overline{c\widetilde{c}} - 2\,\overline{c\delta \widetilde{x}}$$

or

$$\overline{c\widetilde{c}} = G^{-1} - E + 2\,\overline{c\delta \widetilde{x}}$$

However,

$$\overline{c\delta \widetilde{x}} = \overline{\delta x \delta \widetilde{x}} - \overline{\delta m \delta \widetilde{x}} = E - G^{-1}\frac{\partial x}{\partial m}$$

Now (again separating well measured and badly measured variables) using equations

18 and 19 we have

$$\overline{c\delta\widetilde{x}} = \begin{bmatrix} E - G^{-1}\frac{\partial x}{\partial m} & E^c - G^{-1}\frac{\partial x^*}{\partial m} \\ \widetilde{E}^c - G^{*^{-1}}\frac{\partial x}{\partial m^*} & E^* - G^{*^{-1}}\frac{\partial x^*}{\partial m^*} \end{bmatrix}$$

$$= \begin{bmatrix} E^c + G^{-1}(1 + BWBG^{-1}) & E^c + G^{-1}B\widetilde{V} \\ \widetilde{E}^c + G^{*^{-1}}(G^*V\widetilde{B}G^{-1}) & E^* - G^{*^{-1}}(G^*U) \end{bmatrix}$$

or

$$\overline{c\delta\widetilde{x}} = 0 \tag{21}$$

Thus we get

$$\overline{c\widetilde{c}} = G^{-1} - E \tag{22}$$

and have

$$\xi_i = \frac{c_i}{\sqrt{\overline{c_i\widetilde{c_i}}}}$$

For well measured quantities we form c_ic_i in the process of forming E; for badly measured quantities we have

$$\frac{1}{\overline{c\widetilde{c}_{ii}}} = \frac{1}{G_{ii}^{*^{-1}} - E_{ii}^*} = \frac{G_{ii}^*}{1 - G_{ii}^*E_{ii}^*} \tag{23}$$

Resume

Thus, we have a complete procedure. At some point $\bar{x}$, $\bar{x}^*$ we form f, B, and B^* .

Then $r = \widetilde{B}^*\overline{c^*} + \widetilde{B}\overline{c} - f$

and $$H = \widetilde{B}[G^{-1}B]$$

We then solve

$$\begin{pmatrix} -H & \widetilde{B}^* \\ B^* & G^* \end{pmatrix} \begin{pmatrix} \alpha \\ c^* \end{pmatrix} = \begin{pmatrix} r \\ 0 \end{pmatrix}$$

for α and c^*

We then get

$$c = -[G^{-1}B]\alpha$$
$$\chi^2 = -\widetilde{\alpha}r$$

When we have a solution, to calculate errors we form

$$\begin{pmatrix} W & \widetilde{V} \\ V & U \end{pmatrix} = \begin{pmatrix} -H & \widetilde{B}^* \\ B^* & G^* \end{pmatrix}^{-1}$$

Then

$$E = G^{-1} + G^{-1}BW\widetilde{B}G^{-1}$$
$$E^c = -G^{-1}B\widetilde{V}$$
$$E^* = U$$

Finally the pull quantities are calculated by

$$\xi_i = \frac{c_i}{\sqrt{E_{ii} - G_{ii}^{-1}}}$$
$$\xi_i^* = c_i^* \sqrt{\frac{G_{ii}^*}{1 - G_{ii}^* E_{ii}^*}}$$

Criteria for Convergence

It is important to establish criteria for the convergence to a fit. We will require two: 1) the constraints must be satisfied, and 2) X^2 must be at a minimum.

To determine whether the constraints are satisfied we check that the sum of the absolute values of the constraints is small; that is, we form

$$F = \sum_i |f_i| \tag{24}$$

and insist that

$$F < \varepsilon_1 \tag{25}$$

This is done in the subroutine FSSET and ε_1 is stored in FSOK.
If χ^2 is at a minimum, its value will not change. Hence, to check the second condition, we require that

$$|\chi^2 - \overline{\chi^2}| < \varepsilon_2 \tag{26}$$

(ε_2 is stored in DCHIOK)

In the current version of SQUAW $\varepsilon_1 = 0.1$ MeV and $\varepsilon_2 = 0.075$. These parameters, which are set in CONSET, may readily be changed by the user.

Cutting Steps

In our previous derivation we have ignored several problems. First of all, there is no guarantee that when we calculate a new set of variables all these new variables will be physically reasonable. For example, we may form a negative mass or momentum or may find a momentum for a charged track so small that the particle would stop before reaching the end of the track (this is referred to as "overstopped"). In this case we do not wish to use these non-physical variables but instead to use a set of variables that are physically sensible. We then cut the size of the size of the step in an attempt to get reasonable values.

Different aspects of the step cutting procedure are accomplished at different subroutines. The general approach is the following:

If the variables enter a non-physical region the step is cut.

If, after the first step, the constraints don't improve we try a directed step. (See page 85.)

If the directed step doesn't improve the constraints, we retreat to the previous step and try cutting the step.

The subroutines which participate in this and their particular functions are:

XVSET	Locates non-physical variables and sets the flag ICUT appropriately. (Flagged by ICUT= 1, 2, or 3.)
FSSET	Checks the constraint sums and if they are not improving sets the flag ICUT correspondingly. (Flagged by ICUT= 4.)
TEST	Decides whether a solution has been reached or whether another step is necessary.
CUT	Actually cuts the step size for a non-directed step.
NEWVAL	Forms the new values for ordinary or directed steps.
WAMPUM	Supervises by calling out (if ICUT$\neq$0)after XVSET and FSSET and by calling NEWVAL after FSSET (if IFFSTP < 0) and after TEST if a solution hasn't been found (*i.e.* IFAIL < 0).

Description of Step Cutting

For the moment we shall ignore the difference between well measured and badly measured variables. We assume that the approximate values $\bar{x}$ were physically reasonable but that the new values x are not. We may then form new variables x' by cutting the step size by a factor ε.

That is

$$x' = \varepsilon(x - \bar{x}) + \bar{x}$$

or, in terms of the corrections

$$c' = \varepsilon(c - \bar{c}) + \bar{c} = \varepsilon c + (1 - \varepsilon)\bar{c}$$

χ^2 and ψ for Cut Steps

We also wish to calculate the value of χ^2 at the point x'. We have

$$\begin{aligned}\chi^{2'} &= \widetilde{c}' G c' = [\varepsilon\widetilde{c} + (1-\varepsilon)\widetilde{\bar{c}}] G [\varepsilon c + (1-\varepsilon)\bar{c}] \\ &= \varepsilon^2 \widetilde{c} G c + (1-\varepsilon)^2 \widetilde{\bar{c}} G \bar{c} + 2\varepsilon(1-\varepsilon)\widetilde{c} G \bar{c}\end{aligned}$$

We may rewrite this as

$$\chi^{2'} = \varepsilon^2 \chi^2 + (1-\varepsilon)^2 \overline{\chi^2} + 2\varepsilon(1-\varepsilon)\psi \tag{27}$$

where

$$\begin{aligned}\chi^{2'} &= \text{value of } \chi^2 \text{ at point } x' \\ \chi^2 &= \text{value of } \chi^2 \text{ at point } x \\ \overline{\chi^2} &= \text{value of } \chi^2 \text{ at point } \bar{x}\end{aligned}$$

and

$$\psi = \widetilde{c} G \bar{c}$$

Obviously to calculate $\chi^{2'}$ we must know the value of ψ, and if we wish to cut the step size again we must know the value of

$$\psi' = \widetilde{c}' G \bar{c}.$$

This is easily found since

$$\psi' = [\varepsilon\widetilde{c} + (1-\varepsilon)\widetilde{\bar{c}}] G \bar{c} = \varepsilon\psi + (1-\varepsilon)\overline{\chi^2} \tag{28}$$

For a normal step (we now again distinguish between well measured and badly

measured variables) we have

$$\psi = \widetilde{c}^* G^* \bar{c}^* + \widetilde{c} G \bar{c}$$

Upon substituting eq. (14) and (15) we get

$$\begin{aligned}\psi &= (\widetilde{r}\widetilde{V}) G^* \overline{c^*} + (-\widetilde{r} W \widetilde{B} G^{-1}) G \bar{c} \\ &= -\widetilde{r} W \widetilde{B}^* \overline{c^*} - \widetilde{r} W \widetilde{B} \bar{c} \\ &= -(\widetilde{r} W)(\widetilde{B}^* \widetilde{c}^* + \widetilde{B} \bar{c})\end{aligned}$$

or, using equations (8) and (14)

$$\psi = -\widetilde{\alpha}(r + f) \tag{29}$$

Currently ε is set to 1/2. This gives

$$\begin{aligned}c' &= \frac{c + \bar{c}}{2} \\ \chi^{2'} &= \frac{1}{4}\chi^2 + \frac{1}{2}\psi + \frac{1}{4}\overline{\chi^2} \\ \psi' &= \frac{1}{2}(\psi + \overline{\chi^2})\end{aligned}$$

Directed Steps

We may also insist that the constraints improve at each step by insisting that F (eq. 24) become smaller. If instead it becomes larger, it is an indication that the constraints are very non-linear in the region in which we are taking steps.

In this case if we are not near a solution and χ^2 is still changing, we cut the step size, (as before) and check again.* If, however, we are near a minimum for χ^2 (eq. 26 is satisfied) we simply try to take the smallest possible step that will satisfy the constraints.

∗ Solmitz has shown that if we make the step size sufficiently small the constraints are guaranteed to improve (Group A Memo 190).

To do this we define the step size by

$$D = \widetilde{d^*} G^* d^* + dGd \tag{30}$$

where

$$d^* = x^* - \overline{x^*} \tag{31a}$$

$$d = x - \bar{x} \tag{31b}$$

We now introduce Lagrangian multipliers β and define

$$N = 2\widetilde{f}\beta + D = 2\widetilde{f}\beta + \widetilde{d^*} G^* d^* + \widetilde{d} G d \tag{32}$$

We now attempt to minimize N with respect to β, d^*, and d.

The procedure is the same as that used in the normal case to minimize M. We have the relation

$$0 = \frac{1}{2}\frac{\partial N}{\partial \beta} = f(x^*, x) \tag{33a}$$

$$0 = \frac{1}{2}\frac{\partial N}{\partial x^*} = B^*\beta + G^* d^* \tag{33b}$$

$$0 = \frac{1}{2}\frac{\partial N}{\partial x} = B\beta + Gd \tag{33c}$$

We then expand eq. (33a) about the point $(\bar{x}^{\bar{*}},\ \bar{x})$ and, after some algebra, get

$$d = -G^{-1} B\beta \tag{34a}$$

and

$$\begin{pmatrix} -H & \widetilde{B^*} \\ B^* & G^* \end{pmatrix} \begin{pmatrix} \beta \\ d^* \end{pmatrix} = \begin{pmatrix} -f \\ 0 \end{pmatrix} \tag{34b}$$

We may then solve equation (34b) for d^* and β, substitute β in eq. (34a) to find d, and use eq. (31) to get x^* and x.

χ^2 and ψ for Directed Steps

Now

$$\begin{aligned}
\psi &= \widetilde{c}G\bar{c} + \widetilde{c}^*G^*\overline{c^*} \\
&= (\widetilde{\bar{c}} + \widetilde{d})G\bar{c} + (\widetilde{\overline{c^*}} + \widetilde{d^*})G^*\overline{c^*} \\
&= (\widetilde{\bar{c}}G\bar{c} + \widetilde{\overline{c^*}}G^*\overline{c^*}) - \widetilde{\beta}\widetilde{B}G^{-1}G\bar{c} - \widetilde{f}\widetilde{V}G^*\overline{c^*} \\
&= \overline{\chi^2} - \widetilde{\beta}\widetilde{B}\bar{c} + \widetilde{f}W\widetilde{B}^*\overline{c^*} \\
&= \overline{\chi^2} - \widetilde{\beta}(\widetilde{B}\bar{c} + \widetilde{B}^*\overline{c^*})
\end{aligned}$$

or

$$\psi = \overline{\chi^2} - \widetilde{\beta}f - \widetilde{\beta}r \tag{35}$$

Also

$$\begin{aligned}
\chi^2 &= \widetilde{c}Gc + \widetilde{c}^*G^*c^* \\
&= \widetilde{c}G(\bar{c} + d) + \widetilde{c}^*G^*(\overline{c^*} + d^*) \\
&= \psi + (\widetilde{\bar{c}} + \widetilde{d})Gd + (\overline{c^*} + \widetilde{d^*})G^*d^* \\
&= \psi - (\widetilde{\bar{c}} + \widetilde{d})GG^{-1}B\beta - (\overline{c^*} + \widetilde{d^*})G^*Vf \\
&= \psi - (\widetilde{\bar{c}} + \widetilde{d})B\beta + (\overline{c^*} + \widetilde{d^*})B^*Wf \\
&= \psi - (\widetilde{\bar{c}}B + \overline{c^*}B^*)\beta + \widetilde{\beta}\widetilde{B}G^{-1}B\beta + \widetilde{f}\widetilde{V}B^*\beta \\
&= \psi - (\widetilde{f} + r)\beta + \widetilde{f}(\widetilde{V}B^* - WH)\beta \\
&= \psi - \widetilde{r}\beta
\end{aligned}$$

or

$$\chi^2 = \psi - \widetilde{\beta}r = \overline{\chi^2} - \widetilde{\beta}f - 2\widetilde{\beta}r \tag{36}$$

LISET

LISET is entered once for each call to WAMPUM. It sets up lists and initializes data used by WAMPUM. Table 12B gives a list of the data provided by LISET. The vectors and matrices are in WAMCOM (the common block exclusive to WAMPUM)

while the single numbers (counts, *etc.*) are in the common block CONCOM which is common to all of SQUAW. LISET also tests for and sets three values of IFAIL:

IFAIL=30 Dimensions exceeded too many tracks or vertices or coplanarity constraints or inter-track correlations.

IFAIL=31 Too many constraints plus badly-measured variables or too many well-measured variables.

IFAIL=50 Event underdetermined

XVSET

XVSET is called by WAMPUM once for each iteration of a fit. It performs the following functions:

1) Checks to see whether the variables are in the physical region, and, if they are not, it sets the flag for step cutting and failure as follows:

   ICUT=1 negative mass

   ICUT=2 negative curvature

   ICTU=3 overstopped incident track

   IFAIL=15 slope too big

2) Moves current values of variables (NEW) to the vertex (XVERT).

3) At each vertex for incident charged tracks it swims the curvature from the beginning to the end of the track (the end of an incident track is at vertex). Neutral tracks, if they have no connection, are treated like outbound tracks. If they are connected all variables are done at the other end.

4) It calculates derivatives

$$\partial k_e/\partial s_e,\ \partial k_e/\partial s_b,\ \partial k_e/\partial k_b,\ \partial k_e/\partial m \text{ (see description below)}$$

   for the purpose of swimming the curvature. These are stored in DKDK and used also in BFSET to swim the constraint derivatives and in EV?EVFORM to swim the curvature errors to the vertices.

CUT

The subroutine CUT is called by WAMPUM if ICUT$\neq$0. It cuts the step size by 1/2, resets ICUT to zero and counts the numbers of cuts. The following values of IFAIL are set:

IFAIL= 20 Total number of cut-steps too great

IFAIL= 21 Too many successive cut-steps

IFAIL= 51 Tried to cut zeroth step

FKINE

FKINE is called by WAMPUM once for each iteration of a fit. It calculates the constraints (XCOMP) and their derivatives (BEVERT) at each vertex, or interaction point.

In order to evaluate the constraints and their derivatives, we must specify them explicitly. The usual constraints are conservation of energy and momentum at each interaction (*i.e.*, vertex). Thus, we get four constraints for each interaction. They are

$$f_1 = \Sigma_i P_{xi}$$
$$f_2 = \Sigma_i P_{yi}$$
$$f_3 = \Sigma_i P_{zi}$$
$$f_4 = \Sigma_i E_i$$

Clearly, the constraint derivatives for each particle are independent and will depend on the particular set of variables used to parameterize each track.

Thus,

$$\frac{\partial f_i}{\partial x_j} = \frac{\partial P_{xj}}{\partial x_j} \text{ and so on.}$$

Track Type 1

The normal choice of variables is, of course, φ, s, k and m. In this case we have the constraints (stored in XCOMP):

$$
\begin{aligned}
P_{xi} &= (\pm)_i \frac{1}{k_i} \cos\varphi_i \\
P_{yi} &= (\pm)_i \frac{1}{k_i} \sin\varphi_i \\
P_{zi} &= (\pm)_i \frac{1}{k_i} S_i \\
E_i &= (\pm)_i \sqrt{\frac{1+S_i^2}{k_i^2} + m_i^2}
\end{aligned}
$$

Hence, the constraint derivatives (at the interaction point k), BEVERT $(i,\ \lambda,\ k)$ are:

$$
B_{i\lambda} = \frac{\partial f_\lambda}{\partial x_i} = \begin{array}{c} \lambda \\ \downarrow \end{array} \begin{array}{c} \\ \frac{\partial -}{\partial \varphi} \\ \frac{\partial -}{\partial s} \\ \frac{\partial -}{\partial k} \\ \frac{\partial -}{\partial m} \end{array} \begin{array}{c} \begin{array}{cccc} i \rightarrow \frac{\partial Px}{\partial -} & \frac{\partial Py}{\partial -} & \frac{\partial Pz}{\partial -} & \frac{\partial B}{\partial -} \end{array} \\ \begin{pmatrix} -(\pm)_i \frac{1}{k_i} \sin\varphi_i & (\pm)_i \frac{1}{k_i} \cos\varphi_i & 0 & 0 \\ 0 & 0 & (\pm)_i \frac{1}{k_i} & (\pm)_i \frac{S_i}{E_i k_i^2} \\ -(\pm)_i \frac{1}{k_i^2} \cos\varphi_i & -(\pm)_i \frac{1}{k_i^2} \sin\varphi_i & -(\pm)_i \frac{1}{i_{k_{i^2}}} S_i & -(\pm) \frac{1+S_i^2}{E_i k_i^3} \\ 0 & 0 & 0 & (\pm)_i \frac{m_i}{E_i} \end{pmatrix} \end{array}
$$

Track Type 2

In fitting short invisible protons in a deuterium interaction, it is convenient to choose a different set of variables. Here we use the three components of momentum and the mass as the basic variables. These are called "impulse" tracks.

In this case

$$P_{xi} = (\pm)_i P_{xi}$$
$$P_{yi} = (\pm)_i P_{yi}$$
$$P_{zi} = (\pm)_i P_{zi}$$
$$E_i = (\pm)_i \sqrt{P_{xi}^2 + P_{yi}^2 + P_{zi}^2 + m_i^2}$$

Hence, in this case we have BEVERT, $(i,\ \lambda,\ k)$

$$B_{i\lambda} = \frac{\partial f\lambda}{\partial x_i} = \begin{array}{c} \lambda \\ \downarrow \\ \frac{\partial}{\partial p_x} \\ \frac{\partial}{\partial p_y} \\ \frac{\partial}{\partial p_z} \\ \frac{\partial}{\partial m} \end{array} \begin{array}{c} 1 \rightarrow \\ \\ \\ \\ \\ \end{array} \begin{array}{c} \frac{\partial P_x}{\partial -} \\ \\ \\ \\ \\ \end{array} \begin{array}{c} \frac{\partial P_y}{\partial -} \\ \\ \\ \\ \\ \end{array} \begin{array}{c} \frac{\partial P_z}{\partial -} \\ \\ \\ \\ \\ \end{array} \begin{array}{c} \frac{\partial E}{\partial -} \\ \\ \\ \\ \\ \end{array} \begin{pmatrix} (\pm)_i & 0 & 0 & (\pm)_i \frac{P_{xi}}{E_i} \\ 0 & (\pm)_i & 0 & (\pm)_i \frac{P_{yi}}{E_i} \\ 0 & 0 & (\pm)_i & (\pm)_i \frac{P_{zi}}{E_i} \\ 0 & 0 & 0 & (\pm)_i \frac{m_i}{E_i} \end{pmatrix}$$

Track Type 3

For missing mass tracks, we simply use the energy momentum 4-vector as the four variables.

Thus, BEVERT $(i,\ \lambda,\ k)$ at K is

$$B_{i\lambda} = \begin{pmatrix} (\pm)_i & 0 & 0 & 0 \\ 0 & (\pm)_i & 0 & 0 \\ 0 & 0 & (\pm)_i & 0 \\ 0 & 0 & 0 & (\pm)_i \end{pmatrix}$$

FSSET

FSSET forms the sum of the constraints (described in WAMPUM under "criteria for convergence") and tests it. If the constraints have failed to improve it sets ICUT= 4 as an indication to cut the step. It asks whether the constraints are satisfied, whether they are improving, whether a directed step has failed on the previous step, whether a directed step is bad (and therefore we must back up and retake a normal step), and finally whether X^2 is changing sufficiently little to be considered a minimum and hence for the fit to be eligible for a directed step. (Note: A directed step is permitted only if X^2 is at a minimum, otherwise the step must be cut.) The flag IFFST is set in this subroutine as follows:

IFFSTP= -1 take a directed step

IFFSTP= -3 the current directed step is bad, go back to previous normal step (which will subsequently be cut)

BFSET, BEGSET, HHSET

These three subroutines are used to set up the final matrices used in the solution of the equations for new values of the connection to the variables. Recall eqn. 12 of the WAMPUM general description:

$$\begin{pmatrix} -H & \widetilde{B}^* \\ B^* & G^* \end{pmatrix} \begin{pmatrix} \alpha \\ c^* \end{pmatrix} = \begin{pmatrix} r \\ 0 \end{pmatrix}$$

These are finally solved for α and c^* in NEWVAL.

The matrix $\begin{pmatrix} -H & \widetilde{B}^* \\ B^* & G^* \end{pmatrix}$ is stored in HH. BFSET searches through the well and badly measured variables and coplanarity constraints and accumulates and stores the appropriate quantities in the proper parts of HH:B^*, G^*, $\widetilde{B}^*$ and for well measured variables stores $\widetilde{B}$ in BE. BEGSET forms the matrix BEG ($= -G^{-1}B$) and finally HHSET forms the matrix $-H(= \widetilde{B}G^{-1}B)$ and stores it in the appropriate section of HH.

BFSET also forms RR according to eqn. 8 of the WAMPUM description:

$$r = -f + \widetilde{B}^* \bar{c}^* + \widetilde{B}\bar{c}$$

TEST

The primary function of TEST is to see whether a solution has been reached.

That is $F < \varepsilon_1$ or FSOK
and $|\chi^2 - \overline{\chi^2}| < \varepsilon_2$ or DCHIOK

It also counts directed steps and total steps. It resets IFFSTP and NSCUT. TEST sets the following values of IFAIL:

IFAIL= 11 χ^2 too large

IFAIL= 12 too many steps

IFAIL= 22 solution with bad χ^2

NEWVAL

NEWVAL calculates new values of c and c^*, the corrections for well and badly measured variables, respectively.

It does this both for normal steps and for directed steps.

Recall that the expression for normal steps is (eqn. 12 of WAMPUM)

$$\begin{pmatrix} -H & \widetilde{B}^* \\ B^* & G^* \end{pmatrix} \begin{pmatrix} \alpha \\ c^* \end{pmatrix} = \begin{pmatrix} r \\ 0 \end{pmatrix}$$

NEWVAL inquires whether this is to be a directed step (IFFSTP= 3). If so it merely puts $-f$ (stored in FFOLD) into r (stored in RR) and proceeds to solve eqn. 12

of WAMPUM (or 34b for directed steps) for α and c^* (or β and d^* for directed steps). It does this by using the matrix solving subroutine SMXEQU. It then calculates c using eqn. 9 of WAMPUM: $c = G^{-1}B\alpha$, remember that $-G^{-1}B$ was calculated in BEGSET and is stored in BEG. For directed steps it calculates d from β in precisely the same way. If this is a directed step CNEW contains the step and COLD is added to it. Otherwise CNEW is the correction.

Finally the new values of the variables are obtained from the relation:

$$x = m + c.$$

CSQSET

This subroutine calculates χ^2 (stored in CHISQ) and ψ (stored in CHICUT) for both normal and directed steps.

For normal steps it forms

$$\psi = -\widetilde{\alpha}(r + f)$$

and

$$\chi^2 = -\widetilde{\alpha}r$$

For directed steps it uses

$$\psi = \overline{\chi^2} - \widetilde{\beta}f - \widetilde{\beta}r$$

and

$$\chi^2 = \psi - \widetilde{\beta}r$$

See eqns. 18, 29, 35, and 36 of general WAMPUM writeup.

NOTE: There is a diagram of the error storage matrices at the end of this section.

EFORM

EFORM constructs the fitted error matrix EE, and calculates the pull quantities storing them in PULL.

First of all it forms the matrix

$$TT = \begin{pmatrix} W & \widetilde{V} \\ V & U \end{pmatrix} = \begin{pmatrix} -H & \widetilde{B}^* \\ B^* & G^* \end{pmatrix}^{-1}$$

by inventing HH using the matrix inversion subroutine: SMXINV.

It next calculates the temporary quantities PULPK $\left(= \frac{1}{\sqrt{c^* \widetilde{c}^*_{ii}}}\right)$ for badly measured variables.

Then EFORM starts to form the error matrix. This is formed and stored temporarily in EEPK.

The well-measured-well-measured elements:

$$E = G^{-1} + G^{-1} B W \widetilde{B} G^{-1}$$

are, and must be, computed first due to storage consideration. First, EEWS, an intermediate quantity is calculated and stored in a block equivalenced to BE. It then proceeds to form EEPK. This is formed by columns and the column index is the same as that of the EEWS element included in it so that the required column of EEWS is used before it is covered by the ever-expanding EEPK. The program also forms PULPK $(= 1/\sqrt{\overline{c_i^2}})$ for well-measured variables at this point. EFORM then continues to add in the diagonal part of the measurement error, GEE, and the off diagonal part GCOR (*i.e.*, inter-track correlations), storing all in EEPK.

Having finished well measured variables the program calculates well measured-badly measured correlations:

$$E^c = -G^{-1} B V$$

and stores them in EEPK.

Then the badly measured-badly measured elements:

$$E^* = U$$

are moved from TT to EEPK. The temporary quantities EEPK and PULPK are now complete.

Finally EFORM forms

$$\text{PULL} = \text{CNEW}^* \text{ PULPK}$$

and fills the lower triangle of EE from EEPK. It sets both EE and PULL to zero for fixed variables. At the end EE is symmetrized and the fitted error matrix is complete.

CONSET

CONSET sets the values of constants used by SQUAW. It also sets such things as fit and interaction parameters, and storage dimensions used in the calculations. (Do not confuse these with DIMENSION statements.) It sets masses, changes, and the mass identification list.

Since CONSET need only be called once at the beginning of a run it is called by the overall executive program SIOUX when the 6600 version is used. For the 7044/7094 version it is called at the beginning of SQUAW.

CONLEV (CHISQ, NCNSTR)

This is a short function subroutine which is called by TEST. It gives the confidence level as a function of the input parameters CHISQ (χ^2) and NCNSTR (number of constraints). A description of the program is given in the Alvarez Programming Group Memo No. P-347. The only change is that CONLEV has been changed to a function subroutine hence one of the arguments has been eliminated, also the others are rearranged.

Table 5

SQUAW Failures (If IFAIL $\geq$ 30 the event is rejected.)

IFAIL CODES	STATUS OF COUNTERS*	REASON FOR FAILING	FAILING ROUTINE
11	2	χ^2 too high. No fit	TEST
12	2	Too many steps	TEST
13	3	Missing mass below minimum	NONAN
14	3	Outbound track ovestopped at end	NONAN
15	2	Slope exceed maximum allowed	XVSET
16		Not used	
17		Not used	
18		Not used	
19		Not used	
20	2	Too many cut steps	CUT
21	2	Too many successive cut steps	CUT
22	3	Solution with high χ^2	TEST
23	1	Failure of first approximation	APPROX
24	1	Bad track (TP, KPT, or point scatter)	WMSET
25	3	Bad ionization χ^2	BUBBLE
26	2	Equations are singular	NEWVAL
27		Beam track momentum bad	BMAVG
28		Not used	
29		Not used	

30 EVENT REJECTED	1	Too many tracks, vertices, joins correlations	LISET
31		Too many variables	LISET
32		Event type not coded	ETYPE
33		Not used	
34		Too many charge-neutral correlations	DOXTND
35		Too many inter-track correlations	DOXTND
36		Too many tracks or vertices (30)	GOFIT
37		Too many joins (30)	LINK
38		Too many inter-track correlations (35)	
50		Underconstrained	LISET
51	2	Tried to cut zeroth step	CUT
53	3	Singular output error matrix (fit)	EFORM
54	1	Beam error matrix singular	BMAVG
56	1	Illegal LSN type	WMSET
57	1	Input error matrix not positive definite	WMSET

* Certain counters, which are preset in LISET, indicate the path by which the fit is approached. They are ICUT, NSTEP, NCIMPR, NSCUT, IFFSTP, NFFSTP, NTCUT. Their status indicates how meaningful they are for that IFAIL. For all values of IFAIL $\geq$30 (except 51 and 53) the status is 1.

STATUS	(refers to all reject data except mark and reject numbers)
1	No fit. Counters are meaningless, leftover from previous fit.
2	No fit. Counters indicate current value.
3	Fit. Counters indicate situation at time of fit.