Compilation of parameter covariances and sensitivity coefficients

(N. Otsuka, B. Pritychenko, 2025-03-20, Memo CP-D/1129)

A covariance matrix V_z can be decomposed to its uncorrelated part Vx (diagonal matrix) and correlated part V_y.$= S^T M_y S$:

$$V_Z = V_x + V_y = V_x + S\,M_y\,S^T,$$

If there are n data points and the quantity is described by n counts and m parameters (n>>m), the number of non-zero elements of these matrices are n×n for V_Z, n for V_x, n×m for S, and m×m for M_y.

Namely <u>the number of the elements for compilation is reduced from n(n+1)/2 to n + n×m + m(m+1)/2</u> if we adopt the expression of the right-hand side.

When the number of the data points is huge (e.g., 1000) but their uncertainties originate from counts and a few (e.g., 10) parameters, submission of the uncertainties in the counts and covariances of the parameters may significantly reduce the size of the data for our exchange.

Suppose the quantity z at n incident energies is expressed by the number of counts x_i (i=1,n), and parameters y_i (i=1,m):

$$z_i = z_i\,(x_i, y_1, y_2, \ldots, y_m) \tag{1}$$

Its absolute covariance Cov (z_i,z_j) is expressed in terms of Δx_i and Δy_p (p=1,m) by

$$\mathrm{Cov}\,(z_i,z_j) = \delta_{ij}\,(\partial z_i/\partial x_i\,\Delta x_i)^2 + \Sigma_{p,q}\,(\partial z_i/\partial y_p)\,\mathrm{Cov}\,(y_p,y_q)\,(\partial z_i/\partial y_q), \tag{2}$$

where δ_{ij} is Kronecker delta and q=1,m. This demonstrates that the n×n covariances can be expressed by $(\partial z_i/\partial x_i)\,\Delta x_i$, $(\partial z_i/\partial y_p)$ and Cov (y_p,y_q) (i=1,n; p,q=1,m). In this expression, we need to store the following number of elements:

- $(\partial z_i/\partial x_i)\,\Delta x_i$ n elements (statistical uncertainty in z_i)
- $\partial z_i/\partial y_p$ n×m elements (sensitivities)
- Cov (y_p,y_q) m×m elements (symmetric matrix)

The total number of elements is n + n×m + m×(m+1)/2. If there are 1000 incident energies and 10 parameters, then the total number of elements required to express the 1000 × 1000 covariances is reduced from 1000×(1000+1)/2=500500 to 1000 + 10000 + 55 = 11055!

In EXFOR, we can store the $\partial z_i/\partial x_i\,\Delta x_i$ under `ERR-S` and $\partial z_i/\partial y_p$ under `MISC1`, `MISC2`, …, `MISCm`, while Cov (y_p,y_q) can be stored as free text under `COVARIANCE`. If there are more than one counts (e.g., foreground counts and background counts), `ERR-1`, `ERR-2` etc. with the correlation property flag `U` may be used instead of `ERR-S`.

When the z is expressed as a product of m+1 parameters like

$$z_i = x_i\,y_1\,y_2 \ldots y_m \tag{3}$$

and Cov(y_p,y_q) are diagonal, (2) is simplified to

$$\mathrm{cov}\,(z_i,z_j) = \delta_{ij}\,(\delta x_i)^2 + \Sigma_p\,(\delta y_p)^2 \qquad (4)$$

where $\mathrm{cov}(z_i,z_j)=\mathrm{Cov}(z_i,z_j)/(z_i\, z_j)$, $\delta x_i = \Delta x_i/x_i$ and $\delta y_p = \Delta y_p/y_p$. This becomes the **quadrature sum of the partial uncertainties** when i=j.

Example (EXFOR 14836.002 from J.M.Brown+,J,NSE,198,1155,2024)

Transmission at 7030 time-of-flight T(t) is modelled by (1) 2 counts for sample-in $C_s(t)$ and sample-out $C_o(t)$ as well as 10 parameters a, b, k_s, k_o, B_{0s}, B_{0o} and α_i (i=1,4):

$$T(t) = [\alpha_1\, C(E) - \alpha_2\, k_s\, a\, \exp(-bt) - B_{0s}] / [\alpha_3\, C(E) - \alpha_4\, k_o\, a\, \exp(-bt) - B_{0o}]$$

The DATA section contains T, $\Delta_{tot}T$ (total uncertainty), $\Delta_{stat}T$ (statistical uncertainty), and partial derivatives of T in terms of the 10 parameters received from the author in the following form (numbers received from the authors are rounded to four digits after the decimal point for readability):

E	T	$\Delta_{tot}T$	$\Delta_{stat}T$	$\partial T/\partial a$	$\partial T/\partial b$	$\partial T/\partial k_s$	$\partial T/\partial k_o$	$\partial T/\partial B_{0s}$	$\partial T/\partial B_{0o}$	$\partial T/\partial \alpha_1$	$\partial T/\partial \alpha_2$	$\partial T/\partial \alpha_3$	$\partial T/\partial \alpha_4$
eV	no dim.	no dim.	no dim.	?	?	?	?	?	?	?	?	?	?
E	DATA	ERR-T	ERR-S	MISC1	MISC2	MISC3	MISC4	MISC5	MISC6	MISC7	MISC8	MISC9	MISC10
EV	NO-DIM	NO-DIM	NO-DIM	?	?	?	?	?	?	?	?	?	?
150.0312	0.5749	0.1941	0.0772	0.0000	2.9851	-0.8054	0.4588	-0.0093	0.0053	2.4388	-1.3313	-1.6710	0.8636
150.1353	0.6403	0.1291	0.0656	0.0000	1.8091	-0.6246	0.3979	-0.0072	0.0046	2.0866	-1.0325	-1.5922	0.7490
150.2394	0.8181	0.0972	0.0803	0.0000	0.4951	-0.6755	0.5521	-0.0078	0.0064	2.3848	-1.1167	-2.1422	1.0391
150.3437	0.7549	0.0964	0.0700	0.0000	0.9084	-0.6053	0.4560	-0.0070	0.0052	2.1578	-1.0006	-1.8476	0.8583
…	…	…	…	…	…	…	…	…	…	…	…	…	…

with the following definitions of `ERR-T` and `ERR-S` as well as `MISC1` to `MISC10`:

```
MISC-COL   (MISC1)  Derivative of T w.r.t a
           (MISC2)  Derivative of T w.r.t b
           (MISC3)  Derivative of T w.r.t ks
           (MISC4)  Derivative of T w.r.t ko
           (MISC5)  Derivative of T w.r.t B0s
           (MISC6)  Derivative of T w.r.t B0o
           (MISC7)  Derivative of T w.r.t alpha1
           (MISC8)  Derivative of T w.r.t alpha2
           (MISC9)  Derivative of T w.r.t alpha3
           (MISC10) Derivative of T w.r.t alpha4
ERR-ANALYS (ERR-T) Total uncertainty
           (ERR-S) Statistical uncertainty
```

The parameter covariances may be given with short description on how to construct the full covariances ((numbers received from the authors are rounded to four digits after the decimal point for readability):

```
COVARIANCE Full covariance can be derived from the statistical
            uncertainty (ERR-S), sensitivities to the 10
            parameters (MISC1 to MISC10) and the following
            parameter covariances (a1=alpha1 etc.):
           -----------------------------------------------------
               uncertainty  a      b  ks ko B0s B0o a1 a2 a3 a4
           -----------------------------------------------------
           a   3.8349E+02   1
           b   6.0052E-02   0.9931 1
           ks  2.4131E-02   0      0  1
           ko  4.3340E-02   0      0  0  1
           B0s 8.2000E-01   0      0  0  0  1
           B0o 1.0000E+00   0      0  0  0  0   1
           a1  1.0000E-02   0      0  0  0  0   0   1
           a2  1.0000E-02   0      0  0  0  0   0   0  1
           a3  1.0000E-02   0      0  0  0  0   0   0  0  1
           a4  1.0000E-02   0      0  0  0  0   0   0  0  0  1
           -----------------------------------------------------
```