IV.D.1. Derivation of Data Covariance Matrix Equation

In this section, we derive the equation for the data covariance matrix (DCM) in terms of the data-reduction parameters and derivatives with respect to those parameters, as discussed in Section IV.D. See also references [NL04a] and [NL04b]. Readers uninterested in details of the derivation may safely bypass these pages.

Matrix notation is used in this derivation, with indices omitted. We begin with definitions of terms:

- P = theory parameters
  - R-matrix widths & energies, channel radii
  - may also include some measurement-related parameters (Doppler widths, etc.) if not included in p
- p = data-reduction parameter
  - normalization or backgrounds
  - resolution or Doppler widths
  - others
- d = experimental measurement (raw data)
  - related to cross section, but exactly as measured by the experiment
- M = initial covariance matrix for parameters P
  - can be diagonal or off-diagonal
  - can be very large (suggesting little a priori information) or quite small (suggesting the parameters are well known)
- m = initial (measured) covariance matrix for p
  - can be diagonal or off-diagonal
  - are determined during the measurement or data-reduction process
- v = covariance matrix for raw data d
  - no assumption regarding diagonality is made yet, though generally the covariance matrix for measured data is diagonal
- $\tilde{t}$ = theoretical cross section
  - a function of R-matrix parameters in P
  - the quantities whose values are to be determined by this experiment and analysis
- t = theory corresponding to the measured data
  - a function of $\tilde{t}$ and p
- g = partial derivative of theory t with respect to data-reduction parameters p
- G = partial derivative of theory t with respect to theory parameters P

The theory t is a complicated function of the cross section. This function incorporates such effects as beam intensity, duration of the experiment, cosmic and room backgrounds, Doppler- and resolution-broadening, detector dead time, finite-size corrections, and others. The ultimate goal of the measurement and analysis is to learn what that cross section is as a function of energy. In general, one can write

$$t = f\,(\tilde{t}, p) \quad , \qquad \text{(IV D1.1)}$$

where $\tilde{t}$ represents the cross section and p represents any parameters involved in the transformation.

Again we consider Bayes' equations (M+W version), using slightly different notation,

$$\begin{aligned} \mathcal{P}' &= \mathcal{P} + \mathcal{M}'\mathcal{Y} \qquad & \mathcal{M}' &= \left(\mathcal{M}^{-1} + \mathcal{W}\right)^{-1} \\ \mathcal{Y} &= \mathcal{G}^t \mathcal{V}^{-1}\left(\mathcal{D} - \mathcal{T}\right) \qquad & \mathcal{W} &= \mathcal{G}^t \mathcal{V}^{-1} \mathcal{G} \end{aligned} \quad , \qquad \text{(IV D1.2)}$$

where $\mathcal{P}$ represents **all** parameters, $\mathcal{M}$ the full covariance matrix for **all** parameters, $\mathcal{D}$ the measured data, $\mathcal{T}$ the corresponding theoretical calculation, $\mathcal{G}$ the partial derivative of $\mathcal{T}$ with respect to $\mathcal{P}$, and $\mathcal{V}$ the DCM. Primes represent updated values for $\mathcal{P}$ and $\mathcal{M}$. Superscript t, as usual, indicates transpose.

In Eq. (IV D1.2), substitute $\mathcal{D} = d$ and $\mathcal{T} = t$, and $\mathcal{V} = v$; in addition, substitute the matrix identities

$$\mathcal{P} = \begin{bmatrix} P \\ p \end{bmatrix}, \qquad \mathcal{M} = \begin{bmatrix} M & 0 \\ 0 & m \end{bmatrix}, \qquad \mathcal{G} = \begin{bmatrix} G & g \end{bmatrix} \ . \qquad \text{(IV D1.3)}$$

The inverse of $\mathcal{M}$ is then

$$\mathcal{M}^{-1} = \begin{bmatrix} M^{-1} & 0 \\ 0 & m^{-1} \end{bmatrix} \ . \qquad \text{(IV D1.4)}$$

$\mathcal{W} = \mathcal{G}^t \mathcal{V}^{-1} \mathcal{G}$ is therefore found from

$$\mathcal{G}^t \mathcal{V}^{-1} = \begin{bmatrix} G^t v^{-1} \\ g^t v^{-1} \end{bmatrix} \quad \text{and} \quad \mathcal{G}^t \mathcal{V}^{-1} \mathcal{G} = \begin{bmatrix} G^t v^{-1} G & G^t v^{-1} g \\ g^t v^{-1} G & g^t v^{-1} g \end{bmatrix} \ , \qquad \text{(IV D1.5)}$$

so that $\left(\mathcal{M}'\right)^{-1}$ becomes

$$\left(\mathcal{M}'\right)^{-1} = \mathcal{G}^t \mathcal{V}^{-1} \mathcal{G} + \mathcal{M}^{-1} = \begin{bmatrix} G^t v^{-1} G + M^{-1} & G^t v^{-1} g \\ g^t v^{-1} G & g^t v^{-1} g + m^{-1} \end{bmatrix} \ . \qquad \text{(IV D1.6)}$$

$\mathcal{M}'$ is found by inverting that equation. For matrix X of the form

$$X = \begin{bmatrix} A & C^t \\ C & B \end{bmatrix} \ , \qquad \text{(IV D1.7)}$$

the inverse of X can be shown to be

$$X^{-1} = \begin{bmatrix} \left(A - C^t B^{-1} C\right)^{-1} & -\left(A - C^t B^{-1} C\right)^{-1} C^t B^{-1} \\ -\left(B - C A^{-1} C^t\right)^{-1} C A^{-1} & \left(B - C A^{-1} C^t\right)^{-1} \end{bmatrix} \quad , \qquad \text{(IV D1.8)}$$

in which the off-diagonal terms are the transpose of each other:

$$\begin{aligned} \left[\left(B - C A^{-1} C^t\right)^{-1} C A^{-1}\right]^t &= A^{-1} C^t \left(B - C A^{-1} C^t\right)^{-1} \\ &= \left(A - C^t B^{-1} C\right)^{-1} \left(A - C^t B^{-1} C\right) A^{-1} C^t \left(B - C A^{-1} C^t\right)^{-1} \\ &= \left(A - C^t B^{-1} C\right)^{-1} \left[C^t - C^t B^{-1} C A^{-1} C^t\right] \left(B - C A^{-1} C^t\right)^{-1} \qquad \text{(IV D1.9)} \\ &= \left(A - C^t B^{-1} C\right)^{-1} C^t B^{-1} \left[B - C A^{-1} C^t\right] \left(B - C A^{-1} C^t\right)^{-1} \\ &= \left(A - C^t B^{-1} C\right)^{-1} C^t B^{-1} \quad . \end{aligned}$$

That Eq. (IV D1.8) is a correct form for the inverse can readily be verified by calculating $X X^{-1} = X^{-1} X = I$ = the identity matrix, using Eq. (IV D1.9) as necessary.

Substituting the pieces of Eq. (IV D1.6) for $\mathcal{M}'$ into Eq. (IV D1.8) and (IV D1.9) gives

$$\begin{aligned} A - C^t B^{-1} C &= G^t v^{-1} G + M^{-1} - G^t v^{-1} g \left(g^t v^{-1} g + m^{-1}\right)^{-1} g^t v^{-1} G \\ &= G^t \left\{ v^{-1} - v^{-1} g \left(g^t v^{-1} g + m^{-1}\right)^{-1} g^t v^{-1} \right\} G + M^{-1} \qquad \text{(IV D1.10)} \\ &= G^t \left(v + g\, m\, g^t \right)^{-1} G + M^{-1} \quad . \end{aligned}$$

If we then define H as

$$H = v + g\, m\, g^t \quad , \qquad \text{(IV D1.11)}$$

then Eq. (IV D1.10) takes the form

$$A - C^t B^{-1} C = G^t H^{-1} G + M^{-1} \quad . \qquad \text{(IV D1.12)}$$

Analogously, define h as

$$h = v + G\, M\, G^t \quad , \qquad \text{(IV D1.13)}$$

so that

$$B - C A^{-1} C^t = g^t \left(v + G\, M\, G^t \right)^{-1} g + m^{-1} = g^t h^{-1} g + m^{-1} \quad . \qquad \text{(IV D1.14)}$$

Also, since

$$A = G^t v^{-1} G + M^{-1} \quad \text{and} \quad B = g^t v^{-1} g + m^{-1} \quad , \qquad \text{(IV D1.15)}$$

it follows that

$$A^{-1} = M - M\, G^t h^{-1} G\, M \quad \text{and} \quad B^{-1} = m - m\, g^t H^{-1} g\, m \quad . \qquad \text{(IV D1.16)}$$

Making those substitutions into Eq.(IV D1.8) for X^{-1} gives the following for $\mathcal{M}'$:

$$\mathcal{M}' = \begin{bmatrix} \left\{ G^t H^{-1} G + M^{-1} \right\}^{-1} & -\left\{ G^t H^{-1} G + M^{-1} \right\}^{-1} G^t v^{-1} g \\ & \times \left(m - m\, g^t H^{-1} g m \right) \\ -\left\{ g^t h^{-1} g^{-1} + m^{-1} \right\}^{-1} g^t v^{-1} G & \\ \times \left(M - M G^t h^{-1} G M \right) & \left\{ g^t h^{-1} g + m^{-1} \right\}^{-1} \end{bmatrix} . \quad \text{(IV D1.17)}$$

Similarly, for Υ from Eq. (IV D1.2) we find

$$\Upsilon = \begin{bmatrix} G^t v^{-1} (d-t) \\ g^t v^{-1} (d-t) \end{bmatrix} , \quad \text{(IV D1.18)}$$

which leads to

$$\begin{bmatrix} P' - P \\ p' - p \end{bmatrix} = \begin{bmatrix} \left\{ G^t H^{-1} G + M^{-1} \right\}^{-1} G^t v^{-1} (d-t) \ldots \\ -\left\{ G^t H^{-1} G + M^{-1} \right\}^{-1} G^t v^{-1} g \left(m - m\, g^t H^{-1} g\, m \right) g^t v^{-1} (d-t) \\ \\ -\left\{ g^t h^{-1} g + m^{-1} \right\}^{-1} g^t v^{-1} G \left(M - M G^t h^{-1} G M \right) G^t v^{-1} (d-t) \ldots \\ +\left\{ g^t h^{-1} g + m^{-1} \right\}^{-1} g^t v^{-1} (d-t) \end{bmatrix} . \quad \text{(IV D1.19)}$$

Rearranging, this becomes

$$\begin{bmatrix} P' - P \\ p' - p \end{bmatrix} = \begin{bmatrix} \left\{ G^t H^{-1} G + M^{-1} \right\}^{-1} G^t v^{-1} \left\{ 1 - g \left(m - m\, g^t H^{-1} g\, m \right) g^t v^{-1} \right\} \left(d - t \right) \\ \left\{ g^t h^{-1} g + m^{-1} \right\}^{-1} g^t v^{-1} \left\{ -G \left(M - M\, G^t h^{-1} G\, M \right) G^t v^{-1} + 1 \right\} \left(d - t \right) \end{bmatrix}$$

$$= \begin{bmatrix} \left\{ G^t H^{-1} G + M^{-1} \right\}^{-1} G^t v^{-1} \left\{ 1 - g\, m\, g^t v^{-1} + g\, m\, g^t H^{-1} g\, m\, g^t v^{-1} \right\} \left(d - t \right) \\ \left\{ g^t h^{-1} g + m^{-1} \right\}^{-1} g^t v^{-1} \left\{ -G M G^t v^{-1} + G M G^t h^{-1} G M G^t v^{-1} + 1 \right\} \left(d - t \right) \end{bmatrix} \quad \text{(IV D1.20)}$$

$$= \begin{bmatrix} \left\{ G^t H^{-1} G + M^{-1} \right\}^{-1} G^t v^{-1} \left\{ v H^{-1} \right\} (d-t) \\ \left\{ g^t h^{-1} g + m^{-1} \right\}^{-1} g^t v^{-1} \left\{ v h^{-1} \right\} (d-t) \end{bmatrix} ,$$

or

$$\begin{bmatrix} P' - P \\ p' - p \end{bmatrix} = \begin{bmatrix} \left\{ G^t H^{-1} G + M^{-1} \right\}^{-1} G^t H^{-1} (d-t) \\ \left\{ g^t h^{-1} g + m^{-1} \right\}^{-1} g^t h^{-1} (d-t) \end{bmatrix} . \quad \text{(IV D1.21)}$$

Now, consider only the theory parameters *P*. The formulae for these parameters, considered separately from the equations for the data-reduction parameters *p*, take the same form as Bayes' equations, provided that the DCM *V* is replaced by $v + g\, m\, g^t$. Specifically, from Eqs. (IV D1.17) and (IV D1.21), these equations have the form

$$\begin{aligned} &P' - P = M'Y && M' = \left(W + M^{-1}\right)^{-1} \\ &Y = G^t\, H^{-1}\,(d - t) && W = G^t\, H^{-1} G \\ &H = v + g\, m\, g^t && . \end{aligned} \qquad \text{(IV D1.22)}$$

The equations in (IV D1.22) are almost what is needed, except that they are written in terms of the raw data rather than the reduced data (e.g., counts per time channel rather than cross section per energy). Because most analyses are performed in terms of reduced data, it is necessary to convert these equations. If a tilde is used to represent the reduced data, the transformation can be written as

$$\tilde{d} = \tilde{u}\left(d, p\right) \quad . \qquad \text{(IV D1.23)}$$

In Eq. (IV D1.1), we defined *f* as the transformation from "theoretical cross section $\tilde{t}$" to "theory corresponding to measurement *t*". The transformation defined in (IV D1.23) is the inverse of that transformation; that is,

$$\tilde{d} = \tilde{u}\left(d, p\right) = f^{-1}\left(d, p\right) \quad . \qquad \text{(IV D1.24)}$$

Making this transformation everywhere in Bayes' equations for the theory parameters [Eq.(IV D1.22)] will give the equivalent equations in terms of the reduced data rather than the raw data.

This is easily seen in the simple case of a two-parameter data reduction, where parameter *a* is a normalization and *b* a constant background. In this case

$$t = f\,(\tilde{t}, p) = a\,\tilde{t} + b \qquad \text{(IV D1.25)}$$

and

$$\tilde{d} = f^{-1}\,(d, p) = (d - b)/a \quad . \qquad \text{(IV D1.26)}$$

The derivative *G* can therefore be written as

$$G = \frac{\partial t}{\partial P} = a\,\frac{\partial \tilde{t}}{\partial P} = a\,\tilde{G} \quad ; \qquad \text{(IV D1.27)}$$

this equation defines $\tilde{G}$. Likewise, we may define $\tilde{v}$ and $\tilde{g}$ as

$$\tilde{v} = a^{-1}\, v\, a^{-1} \;\text{ and }\; \tilde{g} = a^{-1} g \quad , \qquad \text{(IV D1.28)}$$

and therefore rewrite H in the form

$$H = v + g\ m\ g^t \ = \ a^{-1}\ \tilde{v}\, a^{-1} + a^{-1}\ \tilde{g}\ m\ \tilde{g}^t a^{-1} \ = a^{-1}\ \tilde{H}\ a^{-1} \quad . \tag{IV D1.29}$$

Substituting into Eq. (IV D1.22) for Y and W gives

$$\begin{aligned} Y &= G^{\,t} H^{-1} \left(d - t\right) = \left(\tilde{G}^{\,t} a\right)\left(a^{-1}\tilde{H}^{-1} a^{-1}\right)\left(a\,\tilde{d} + b - a\,\tilde{t} - b\right) \\ &= \tilde{G}^{\,t} \tilde{H}^{-1}\left(\tilde{d} - \tilde{t}\right) \end{aligned} \tag{IV D1.30}$$

and

$$W = G^{\,t} H^{-1} G = \left(\tilde{G}^{\,t} a\right)\left(a^{-1}\tilde{H}^{-1} a^{-1}\right)\left(a\,\tilde{G}\right) = \tilde{G}^{\,t}\tilde{H}^{-1}\tilde{G} \quad . \tag{IV D1.31}$$

The form of the equation is the same, with or without tildes.

In the general case, equations analogous to (IV D1.25) and (IV D1.26) are

$$\begin{aligned} \tilde{t} &= \tilde{u}\left(x, p\right) \quad \text{at} \quad x = t \\ \text{or} \quad t &= f\left(\tilde{x}, p\right) \quad \text{at} \quad \tilde{x} = \tilde{t} \end{aligned} \tag{IV D1.32}$$

and

$$\begin{aligned} \tilde{d} &= \tilde{u}\left(x, p\right) \quad \text{at} \quad x = d \\ \text{or} \quad d &= f\left(\tilde{x}, p\right) \quad \text{at} \quad \tilde{x} = \tilde{d} \quad . \end{aligned} \tag{IV D1.33}$$

The function $\tilde{u}$ is the inverse of the function f :

$$\begin{aligned} x &= f\left(\tilde{x}, p\right) = f\left(\tilde{u}\left(x, p\right), p\right) \\ \text{or} \quad \tilde{x} &= \tilde{u}\left(x, p\right) = \tilde{u}\left(f\left(\tilde{x}, p\right), p\right) \quad . \end{aligned} \tag{IV D1.34}$$

Relationships between various partial derivatives can be established by using the chain rule,

$$1 = \frac{\partial x}{\partial x} = \frac{\partial f\left(\tilde{u}\left(x, p\right), p\right)}{\partial x} = \frac{\partial f\left(\tilde{x}, p\right)}{\partial \tilde{x}}\ \frac{\partial \tilde{u}\left(x, p\right)}{\partial x} \tag{IV D1.35}$$

or

$$\frac{\partial \tilde{u}\left(x, p\right)}{\partial x} = \left[\frac{\partial f\left(\tilde{x}, p\right)}{\partial \tilde{x}}\right]^{-1} \quad . \tag{IV D1.36}$$

Note that both $\tilde{t}$ and d are independent of the data-reduction parameters p: $\tilde{t}$ is calculated directly from the theory parameters P, and d is measured directly with no corrections. Therefore, the following relationships hold:

$$0 \ = \ \frac{\partial d}{\partial p} \ = \ \left.\frac{\partial f}{\partial p}\right|_{\tilde{x}=\tilde{d}} + \left.\frac{\partial f}{\partial \tilde{x}}\right|_{\tilde{x}=\tilde{d}} \left.\frac{\partial \tilde{u}}{\partial p}\right|_{x=d} \tag{IV D1.37}$$

and

$$0 \;=\; \frac{\partial \tilde{t}}{\partial p} \;=\; \left.\frac{\partial \tilde{u}}{\partial p}\right|_{x=t} + \left.\frac{\partial \tilde{u}}{\partial x}\right|_{x=t} \left.\frac{\partial f}{\partial p}\right|_{\tilde{x}=\tilde{t}} \quad . \tag{IV D1.38}$$

The last term, however, is exactly equal to our definition of g at the beginning of this section.

We now consider a Taylor expansion of $d = f\left(x, p\right)\big|_{x=\tilde{d}}$ in the neighborhood of $\tilde{t}$, for fixed p:

$$d = f\left(\tilde{d}, p\right) \approx f\left(\tilde{t}, p\right) + \left.\frac{\partial f}{\partial \tilde{x}}\right|_{\tilde{x}=\tilde{t}} \left\{\tilde{d} - \tilde{t}\right\} \approx t + \left.\frac{\partial f}{\partial \tilde{x}}\right|_{\tilde{x}=\tilde{t}} \left\{\tilde{d} - \tilde{t}\right\} \quad . \tag{IV D1.39}$$

For simplicity, define F as

$$F = \left.\frac{\partial f}{\partial \tilde{x}}\right|_{\tilde{x}=\tilde{t}} \quad ; \tag{IV D1.40}$$

it follows that

$$d - t \;=\; t + F\left\{\tilde{d} - \tilde{t}\right\} - t \;=\; F\left\{\tilde{d} - \tilde{t}\right\} \quad . \tag{IV D1.41}$$

In similar fashion, the derivative with respect to the R-matrix parameters can be written as

$$G \;=\; \frac{\partial t}{\partial P} \;=\; \frac{\partial t}{\partial \tilde{t}} \frac{\partial \tilde{t}}{\partial P} \;=\; F\,\tilde{G} \quad . \tag{IV D1.42}$$

Substituting those expressions into Eq. (IV D1.22) for Y and W gives

$$Y = G^{t} H^{-1}\left(d - t\right) = \left(\tilde{G}^{t} F^{t}\right) H^{-1} F\left\{\tilde{d} - \tilde{t}\right\} = \tilde{G}^{t} F^{t} H^{-1} F\left\{\tilde{d} - \tilde{t}\right\} \tag{IV D1.43}$$

and

$$W = G^{t} H^{-1} G = \left(\tilde{G}^{t} F^{t}\right) H^{-1}\left(F\,\tilde{G}\right) = \tilde{G}^{t} F^{t} H^{-1} F\,\tilde{G} \quad . \tag{IV D1.44}$$

Inserting the definition of H from Eq. (IV D1.11) gives

$$\begin{aligned} F^{t} H^{-1} F &= \left(F^{-1} H \left(F^{t}\right)^{-1}\right)^{-1} = \left(F^{-1}\left\{v + g\,m\,g^{t}\right\}\left(F^{t}\right)^{-1}\right)^{-1} \\ &= \left(F^{-1} v \left(F^{t}\right)^{-1} + F^{-1} g\,m\,g^{t}\left(F^{t}\right)^{-1}\right)^{-1} \\ &= \left(F^{-1} v \left(F^{t}\right)^{-1} + \left(F^{-1} g\right) m \left(F^{-1} g\right)^{t}\right)^{-1} \quad , \end{aligned} \tag{IV D1.45}$$

so that *Y* and *W* can be written in the desired form,

$$Y = \tilde{G}^t \, \tilde{H}^{-1} \left\{ \tilde{d} - \tilde{t} \right\} \qquad \text{(IV D1.46)}$$

and

$$W = \tilde{G}^t \, \tilde{H}^{-1} \, \tilde{G} \quad , \qquad \text{(IV D1.47)}$$

provided $\tilde{H}$ is defined as

$$\tilde{H} = F^{-1} H \left(F^t\right)^{-1} = F^{-1} v \left(F^t\right)^{-1} + \left(F^{-1} g\right) m \left(F^{-1} g\right)^t \quad . \qquad \text{(IV D1.48)}$$

If we then invoke Eqs. (IV D1.36), (IV D1.38), and (IV D1.40), the expression for $F^{-1}g$ in Eq. (IV D1.48) can be written as

$$F^{-1} g = \left.\frac{\partial \tilde{u}}{\partial x}\right|_{x=t} \left.\frac{\partial f}{\partial p}\right|_{\tilde{x}=\tilde{t}} = -\left.\frac{\partial \tilde{u}}{\partial p}\right|_{x=t} \quad , \qquad \text{(IV D1.49)}$$

which yields

$$\begin{aligned} \tilde{H} &= F^{-1} \quad v \left(F^t\right)^{-1} \quad + \quad \left(F^{-1} g\right) \quad m \quad \left(F^{-1} g\right)^t \\ &= \left.\frac{\partial \tilde{u}}{\partial x}\right|_{x=t} v \left.\frac{\partial \tilde{u}}{\partial x}\right|_{x=t} + \left(-\left.\frac{\partial \tilde{u}}{\partial p}\right|_{x=t} \right) m \left(-\left.\frac{\partial \tilde{u}}{\partial p}\right|_{x=t} \right)^t \end{aligned} \qquad \text{(IV D1.50)}$$

or

$$\tilde{H} = \left.\frac{\partial u}{\partial x}\right|_{x=t} v \left.\frac{\partial \tilde{u}}{\partial x}\right|_{x=t} + \left.\frac{\partial \tilde{u}}{\partial p}\right|_{x=t} m \left(\left.\frac{\partial \tilde{u}}{\partial p}\right|_{x=t} \right)^t \quad . \qquad \text{(IV D1.51)}$$

Bayes' equations can therefore be written in the form

$$\begin{aligned} &P' - P = M'Y && M' = \left(W + M^{-1}\right)^{-1} \\ &Y = \tilde{G}^t \, \tilde{H}^{-1} \left(\tilde{d} - \tilde{t}\right) && W = \tilde{G}^t \, \tilde{H}^{-1} \tilde{G} \\ &\tilde{H} = \tilde{v} + \tilde{g} \, m \, \tilde{g}^t \quad , \end{aligned} \qquad \text{(IV D1.52)}$$

in which we have defined $\tilde{v}$ and $\tilde{g}$ as

$$\tilde{v} = \left.\frac{\partial u}{\partial x}\right|_{x=t} v \left.\frac{\partial \tilde{u}}{\partial x}\right|_{x=t} \quad \text{and} \quad \tilde{g} = \left.\frac{\partial \tilde{u}}{\partial p}\right|_{x=t} \quad . \qquad \text{(IV D1.53)}$$

We now consider how $\tilde{H}$ is related to the covariance matrix for the reduced data (i.e., for $\tilde{d}$). The covariance matrix for the reduced data is customarily found from

$$\begin{aligned}\tilde{V} &= \langle \delta\tilde{d}\ \delta\tilde{d} \rangle = \left.\frac{\partial \tilde{u}}{\partial x}\right|_{x=d} \langle \delta d\ \delta d \rangle \left.\frac{\partial \tilde{u}}{\partial x}\right|_{x=d} + \left.\frac{\partial \tilde{u}}{\partial p}\right|_{x=d} \langle \delta p\ \delta p \rangle \left.\frac{\partial \tilde{u}}{\partial p}\right|_{x=d} \\ &= \left.\frac{\partial \tilde{u}}{\partial x}\right|_{x=d} v \left.\frac{\partial \tilde{u}}{\partial x}\right|_{x=d} + \left.\frac{\partial \tilde{u}}{\partial p}\right|_{x=d} m \left.\frac{\partial \tilde{u}}{\partial p}\right|_{x=d} .\end{aligned} \tag{IV D1.54}$$

In this form, $\tilde{V}$ in Eq. (IV D1.54) is very similar to $\tilde{H}$ of Eq. (IV D1.51). The only difference between the two is the value at which the derivatives are evaluated, that is, at $x = t$ for $\tilde{H}$ and $x = d$ for the usual $\tilde{V}$. It therefore follows that the only modification needed in the "usual" definition of data covariance matrix is to evaluate the various terms at the theoretical values, not the experimental values.

Conclusion

Exact agreement between the fit-to-raw-data method and the fit-to-reduced-data method is obtained by evaluating partial derivatives at the "true" cross section values (theoretical cross section values) rather than at the measured (experimental) values.

The agreement is exact only for first-order fitting, without iteration for nonlinearities.