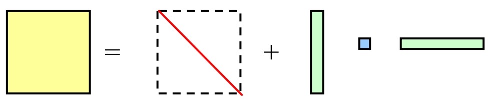
IV.D.3. Implicit Data Covariance Matrix

As seen in previous sections, Bayes' Equations for updating parameter and covariance matrices require the inversion of the data covariance matrix (DCM) V. Because the dimension of V can be very large (~1000's), performing this inversion explicitly can consume significant computer resources (CPU time and memory). Results can also be inaccurate, due to the round-off errors that occur when dealing with such a large quantity of numbers. Fortunately, there is an alternative method that is far more efficient than explicit calculation and inversion of V. This alternative method is denoted the Implicit Data Covariance (IDC) method.

As demonstrated in Section IV.D.1, the DCM can be written as a sum of two terms. The first, v, is a diagonal portion that contains statistical errors due to the measurement itself. The second term, $g\,m\,g^t$, characterizes the uncertainties in the data-reduction process; these are called systematic or common errors, since they apply systematically to all data points. This term is, in general, fully off-diagonal.

In matrix notation, the formula for the DCM is

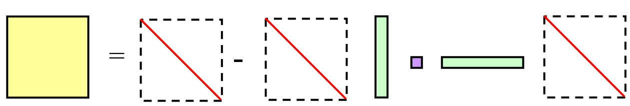
$$V = v + g\;m\;g^t \qquad \text{(IV D3.1)}$$



Here the boxes* are intended to represent the size of the matrices and are best viewed logarithmically. The dimensions of V may be quite large (~ tens or hundreds of thousands), and the dimensions of m are generally quite small (~ tens). Solid boxes represent full (non-diagonal) matrices; a dashed box indicates a diagonal matrix.

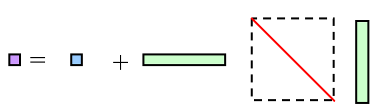
Because V has the form shown above, the inverse may be calculated symbolically as

$$\begin{aligned} V^{-1} &= \left(v + g\,m\,g^t\right)^{-1} \\ &= v^{-1} - v^{-1} g \left(m^{-1} + g^t v^{-1} g\right)^{-1} g^t v^{-1} \qquad \text{(IV D3.2)} \\ &= v^{-1} - v^{-1}\; g\; Z^{-1}\; g^t\; v^{-1} \;, \end{aligned}$$



in which Z is given by

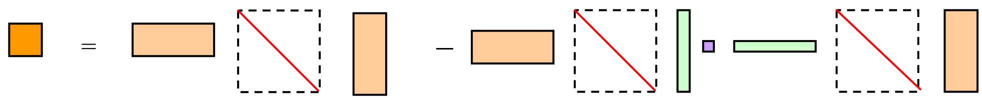
$$Z = m^{-1} + g^t\; v^{-1}\; g \;. \qquad \text{(IV D3.3)}$$



* Thanks to Helmut Leeb for suggesting this method of visualization.

Equations (IV D3.2) and (IV D3.3) provide an easy way to generate the inverse of the DCM. However, further simplification is possible. It is not V^{-1} that is needed, but the product of V^{-1} with other quantities. In particular, for the M+W version of Bayes' equations, matrices W and Y are needed. The expression for W may be written as follows:

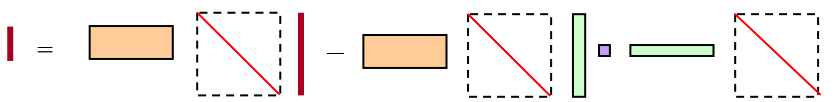
$$\begin{aligned} W &= G^t \quad V^{-1} \quad G \\ &= G^t \quad v^{-1} \quad G \quad - \quad G^t \quad v^{-1} \quad g \;\; Z^{-1} \;\; g^t \quad v^{-1} \quad G \; . \end{aligned} \qquad \text{(IV D3.4)}$$



In this expression, a third dimension has been added, this being the number of varied parameters (~ hundreds or thousands). Typically, this is intermediate between the number of data points and the number of data-reduction parameters.

The expression for Y is

$$\begin{aligned} Y &= G^t \quad V^{-1}\left(D-T\right) \\ &= G^t \quad v^{-1}\left(D-T\right) \quad - \quad G^t \quad v^{-1} \quad g \;\; Z^{-1} \;\; g^t \quad v^{-1}\left(D-T\right) \end{aligned} \qquad \text{(IV D3.5)}$$



The new dimension introduced in this expression is 1, since $D - T$ and Y are simple vectors.

On first inspection, the expressions in the second lines of Eqs. (IV D3.4) and (IV D3.5) appear to be more complicated than the original expressions in the first lines. Indeed, they are somewhat more complicated to program. However, there are significant advantages to using the second expressions: The only large matrix, v^{-1}, is diagonal and therefore trivial to compute. The other two matrices that must be inverted, m and Z, are both very small (and m is often diagonal). Thus computation time is reduced because no large dense matrix is ever inverted. The required computer memory is reduced because no large matrix is ever stored. Finally, numerical accuracy and stability are improved because there are fewer opportunities to encounter round-off problems.

See papers [NL04a] and [NL04b] for computational verification of the claims made in the preceding paragraph. For the example cited in those papers, computation time for solving Bayes' equations was reduced by a factor of ~300 and array size by a factor of ~6 when using the IDC method. Accuracy was also improved, as great care is needed to ensure that sufficient significant digits are provided when using an explicit DCM.

Several options are available in SAMMY for using the IDC method. The earliest available form was restricted to normalization and background corrections. See Section III.E.3

for a discussion of these corrections and Section VI.C.3.c for a description of the original IDC-relevant input. For the release of sammy-7.0.0 in 2006, two additional options were made available: The first is the PUP option, discussed in Sections IV.D.1 and IV.D.2. The second is for the user to provide externally generated values for *g* and *m*. Input details are provided in Section VI.C.3.b.