the neglected error dependency between two datasets might become much larger than the smaller error covariance, e.g., $\Delta\mathbf{D}_{\widetilde{k};\widetilde{i}} - \Delta\mathbf{D}_{\widetilde{j};\widetilde{k}} \approx 0$, $\frac{1}{2}\Delta\mathbf{D}_{\widetilde{i};\widetilde{j}} > \mathbf{C}_{\widetilde{i}}\big|_{\text{true}}$. This phenomena was also described and demonstrated by Sjoberg et al. (2021) for scalar problems, but the generalization to covariances matrices is expected to increase the occurrence of negative values in off-diagonal elements. Because spatial correlations and, thus, true covariances may become small compared with uncertainties in the assumptions or sampling noise, estimated error covariances at these locations might become negative. However, the occurrence of negative elements does not affect the positive definiteness of a covariance matrix, which is determined by the sign of its eigenvalues.

4.2 Approximation for more than three datasets

While independence among all datasets is required to estimate the error covariances of three datasets ($I = 3$), the use of more than three datasets ($I > 3$) enables the additional estimation of some error dependencies or cross-covariances (see Sect. 2)CE6. Although this potential of cross-statistic estimation was previously indicated by Gruber et al. (2016) and Vogelzang and Stoffelen (2021) for scalar problems, a generalized formulation exploiting its full potential by minimizing the number of assumptions is still missing.

As described in Sect. 2 for $I > 3$ datasets, $A_I > 0$ gives the number of error cross-statistics that can potentially be estimated in addition to all error covariances. Consequentially, the independence assumption between all pairs of datasets can be relaxed to a "partial-independence assumption" where one independent dataset pair is required for each dataset I. The estimation of error covariances can be generalized in two ways. Firstly, the direct formulation for three datasets in Sect. 4.1.1 is generalized to a direct estimation of more than three datasets in Sect. 4.2.1. Secondly, Sect. 4.2.2 introduces the sequential estimation of error covariances of any additional dataset. This estimation procedure of additional error covariances is denoted as "sequential estimation", as it requires the error covariance estimate of a prior dataset, in contrast to the "direct estimation" from an independent triplet of datasets ("triangular estimation" in Sect. 4.1) or generally from a closed series of pairwise independent datasets ("polygonal estimation" in Sect. 4.2.1).

4.2.1 Direct error covariance estimates

For more than three datasets ($I > 3$), the estimation from three residual covariances in Eq. (39) can be generalized to estimations of error covariances from a closed series of F residual covariances (see Sect. 3.3.1). For any odd F with $3 \le F \le I$, each error covariance can be estimated under the assumption of vanishing error dependencies along the closed series of datasets $\mathbf{D}_{\widetilde{i_f};\widetilde{i_{f+1}}}\ \forall f \in [1, F-1]$ and $\mathbf{D}_{\widetilde{i_F};\widetilde{1}}$:

$$\mathbf{C}_{\widetilde{i_1}} \overset{(29)}{\underset{\{\text{in}F\}}{\approx}} \frac{1}{2}\left[\left(\sum_{f=1}^{F-1}(-1)^{f-1}\boldsymbol{\Gamma}_{i_f;i_{f+1}}\right) + \boldsymbol{\Gamma}_{i_F;i_1}\right],$$
$$\forall F \text{ odd } \wedge 3 \le F \le I. \tag{48}$$

Here, "$\underset{\{\text{in}F\}}{\approx}$" indicates the assumption of neglectable error dependencies along the series of datasets. As shown in Sect. 2, the problem cannot be closed for less than three datasets, even under the independence assumption. For $F = 3$ datasets, Eq. (39) is a special case of Eq. (48) with indices $i_1 = i$, $i_2 = j$, and $i_3 = k$.

4.2.2 Sequential error covariance estimates

Similar to the estimation for three datasets ($I = 3$) in Sect. 4.1.1, the error covariances of the first three datasets can be directly estimated from residual covariances or cross-covariances using Eqs. (39), (40), or (41). This triplet of the first three datasets that are assumed to be pairwise independent is denoted as a "basic triangle". Similarly, a "basic polygon" can be defined from a closed series of F pairwise independent datasets, where each two successive datasets in the series as well as the last and first element are independent of each other (see Sect. 4.2.1). Then, the error covariance of each dataset in the series can be directly estimated from Eq. (48).

Based on this, the remaining error covariances can be calculated sequentially. For each additional dataset i with $F < i < I$CE7, its cross-statistics to one prior dataset $\text{ref}(i) < i$ need to be assumed in order to close the problem. This prior dataset $\text{ref}(i)$ is denoted as the "reference dataset" of dataset i. With this, the remaining error covariances can be estimated from residual covariances under the partial-independence assumption $\mathbf{X}_{\widetilde{i};\widetilde{\text{ref}(i)}} = 0$:

$$\mathbf{C}_{\widetilde{i}} \overset{(25)}{\underset{\{\text{in}I\}}{\approx}} \boldsymbol{\Gamma}_{i;\text{ref}(i)} - \mathbf{C}_{\widetilde{\text{ref}(i)}}, \tag{49}$$

where "$\underset{\{\text{in}I\}}{\approx}$" indicates the assumption of independence to the reference dataset, i.e., $\mathbf{X}_{\widetilde{i};\widetilde{\text{ref}(i)}} = 0$.

Similarly, each additional error covariance can be estimated from two residual cross-covariances with respect to its reference dataset $\text{ref}(i)$ and any other dataset j:

$$\mathbf{C}_{\widetilde{i}} \overset{(34)}{\underset{\{\text{in}I\}}{\approx}} \boldsymbol{\Gamma}_{i;\text{ref}(i);i;j} + \boldsymbol{\Gamma}_{\text{ref}(i);i;\text{ref}(i);j} - \mathbf{C}_{\widetilde{\text{ref}(i)}}. \tag{50}$$

From the equivalence of residual statistics in Eq. (35), it follows that the two formulations of error covariances in Eqs. (49) and (50), respectively, are equivalent and produce exactly the same estimates, even if the underlying assumptions are not perfectly fulfilled.