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Published Version

Fowler, A. M. ORCID: https://orcid.org/0000-0003-3650-3948 (2024) On the robustness of methods to account for background bias in data assimilation to uncertainties in the bias estimates. Quarterly Journal of the Royal Meteorological Society, 150 (763). pp. 3657-3671. ISSN 1477-870X doi: 10.1002/qj.4790 Available at https://centaur.reading.ac.uk/116845/

To link to this article DOI: http://dx.doi.org/10.1002/qj.4790

Publisher: Royal Meteorological Society

Received: 8 February 2024 | Revised: 3 May 2024 | Accepted: 4 June 2024

DOI: 10.1002/qj.4790

RESEARCH ARTICLE

Quarterly Journal of the Royal Meteorological Society RMetS

On the robustness of methods to account for background bias in data assimilation to uncertainties in the bias estimates

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Funding information
National Centre for Earth Observation, Grant/Award Number: PR140015

Abstract

Fundamental to the theory of data assimilation is that the data (i.e., the observations and the background) provide an unbiased estimate of the true state. There are many situations when this assumption is known to be far from valid; and without bias correction (BC), significant biases will be present in the resulting analysis. Here, we compare two methods to account for biases in the background that do not require a change to the data assimilation algorithm: explicit BC and covariance inflation (CI). When the background bias is known perfectly it is clear that the BC method outperforms the CI method, in that it can completely remove the effect of the background bias whereas the CI method can only reduce it. However, the background bias can only be estimated when unbiased observations are available. A lack of unbiased observations means that the estimate of the background bias will always be subject to sample errors and structural errors due to poor assumptions about how the bias varies in space and time. Given these difficulties in estimating the background bias, the robustness of the two methods in producing an unbiased analysis is studied within an idealised linear system. It is found that the CI method is much less sensitive to errors in the background bias estimate and that a smooth estimate of the bias is crucial to the success of the BC method. However, the CI method is more sensitive to uncorrected biases in the observations.

KEYWORDS

covariance inflation, offline bias correction

1 | INTRODUCTION

Data assimilation, the systematic blending of observations with models, has proven to be essential to the skill of modern-day numerical weather prediction, and its potential in other areas of geophysics is now increasingly being realised Carrassi *et al.* (2018). Fundamental to the theory of data assimilation is that the observations and the background (the best guess of the model state, usually given by a previous forecast) provide an unbiased estimate of the true state. The assimilation of unbiased data will then provide a new estimate of the state (known as the analysis) that is also unbiased. Therefore, the problem of data assimilation can be formulated in terms of finding the state with the minimum error covariance (Kalnay, 2003). Unfortunately, there are many situations when the biases in the background and observations are far from negligible; therefore, the analysis will also be biased.

Here, we concentrate solely on correcting biases in the background, assuming (rightly or wrongly) that the observations are unbiased—possibly because the observations are of relatively high quality, have been carefully bias-corrected before assimilation, or an online bias correction (BC) method Auligné *et al.* (2007) has successfully been implemented). The background biases may be caused by systematic errors in the numerical model propagating the analysis from the previous assimilation cycle to become the background at the current assimilation cycle, as well as biases in the previous analysis itself. The biases in the model arise due to missing physical processes, inadequate parametrisations, or systematic errors in the boundary forcing, to name but a few. The complex sources of the bias that manifests in the background mean that it can be difficult to untangle them, and the background bias may vary in time and space (Bonavita *et al.*, 2012).

Two general approaches that could be taken to reduce the bias in the analysis are:

- If the biases are known then they may be removed from the background before assimilation, without attempting to correct the source of the bias.
- If the biases are known then they may be used to inflate the background error covariances, resulting in the unbiased observations having more weight—as discussed in Dee and Da Silva (1998). We shall refer to this method hereafter as "covariance inflation" (CI).

A third approach could be to perform anomaly correction so that the model climatology is maintained during the assimilation. This has the advantage of avoiding shocks due to the assimilation of observations and the information loss as the model returns to its climatology (Smith *et al.*, 2013). Post-processing can then be used to remove the bias thereafter. This approach has gained popularity in seasonal forecasting but has fewer advantages when interested in shorter lead times. As such, in the remainder of this article we focus on the first two approaches.

If the biases are known *exactly* then explicit BC is the most optimal approach to providing an unbiased analysis, whereas the CI approach can only reduce the bias in the analysis and is done so at the expense of increasing the random error in the analysis, as will be discussed further in Section 2.2. Explicit BC has therefore been the more typical approach to treating background biases (e.g., Lea *et al.*, 2008; Laloyaux *et al.*, 2020). The potential for CI has, however, been acknowledged in a few applications, but it is generally seen as a "blunt tool" to bias reduction and is applied somewhat ad hoc, as stated by Bonavita and Laloyaux (2020). For example, in the ensemble Kalman filter, the use of CI is common to counteract problems with undersampling due to the limited sample size but has also been shown to reduce analysis bias (Raanes *et al.*, 2019). Often, the inflation is based on a simple scaling factor and is unable to consider the spatial structure of the bias (Anderson, 2009; Miyoshi *et al.*, 2010). Alternatively, the inflation is generated using different random realisations of model error in each ensemble member, encapsulating the random model error but not explicitly the bias. For a review of the different approaches to CI in the ensemble Kalman filter, see Houtekamer and Zhang (2016). In contrast, within the UK Met Office's implementation of ocean data assimilation via NEMOVAR, the background error correlations are modelled as the sum of two Gaussians, one with a longer length scale to allow for a correction of large-scale errors due to atmospheric forcing (Mirouze *et al.*, 2016). Again, this is a very simple way of addressing the bias and does not address spatial and temporal variations in the background bias. It has also been shown to sometimes cause problems when assimilating sparse subsurface profile observations. The use of CI to explicitly account for significant background biases was applied to marine biogeochemistry data assimilation by Fowler *et al.* (2022) on the northwest European Shelf seas. They found that the skill of the analysis and forecast was very sensitive to the use of CI and could cause large degradations as well as improvements. They concluded that this sensitivity may be due to the coarse binning of the bias when applying the CI and, as such, the estimated bias did not give a good representation of the bias characteristics in all regions across the complex domain of the shelf seas.

In practice, the background bias can be estimated from a historic sample of innovations (observation–background differences). However, these will always be limited to where high-quality, unbiased observations are available. To reduce sampling error, assumptions about ergodicity and homogeneity need to be imposed, which will limit the amount of detail that can be provided about how the bias varies in space and time. Methods to learn the bias online, such as weak-constraint four dimensional variational data assimilation (WC-4DVar Laloyaux *et al.*, 2020), have also been developed but are still constrained by the available data and assumptions about how the biases vary in space and time.

Given the difficulty in estimating the background bias, this article aims to compare the performance of explicit BC and CI in reducing the biases in the analysis state in the case when the properties of the biases are only approximately known. The robustness of each method to sample and/or structural errors in the estimate of the bias is explored. In Section 2 we first present the theory for how the biases in the background propagate through to the analysis and the impact this has on the analysis mean-square error (MSE) when the bias is unaccounted for and when it is accounted for using explicit BC (Section 2.1) and using CI (Section 2.2). In Section 2.3 the problem of estimating the bias in the background is discussed and the necessary trade-off between the sample size and the number of parameters used to model the bias. In Section 3 numerical results are presented to demonstrate how robust the two different approaches to BC are to uncertainties in the estimate of the bias. Experiments are performed when all observations are unbiased as well as when one instrument has a systematic error in measuring the same variable.

2 | THEORY

We first present the general theory for when no attempt is made to correct the biases in the data.

In variational data assimilation, the analysis of the state at time i is found by minimising the following cost function with respect to the state $\mathbf{x}^i \in \mathbb{R}^n$:

$$J(\mathbf{x}^i) = (\mathbf{x}^i - \mathbf{x}_\mathrm{b}^i)^\mathrm{T}(\mathbf{B}^i)^{-1}(\mathbf{x}^i - \mathbf{x}_\mathrm{b}^i) + \left(\mathbf{y}^i - h(\mathbf{x}^i)\right)^\mathrm{T}(\mathbf{R}^i)^{-1}\left(\mathbf{y}^i - h(\mathbf{x}^i)\right), \quad (1)$$

where $\mathbf{y}^i \in \mathbb{R}^{p_i}$ are the observations relevant to $\mathbf{x}^i$ and $h(\cdot) : \mathbb{R}^n \rightarrow \mathbb{R}^{p_i}$ is the vector function mapping the state variables to those observed (this may include interpolation to account for differences in location of the observations to the model grid, a change of variables, or a dynamical model to account for observations at different times). $\mathbf{R}^i \in \mathbb{R}^{p_i \times p_i}$ is the observation error covariance matrix. $\mathbf{x}_\mathrm{b}^i \in \mathbb{R}^n$ is the background state vector at time i, and $\mathbf{B}^i \in \mathbb{R}^{n\times n}$ is the background error covariance matrix.

The analysis that minimises Equation (1) is the state with the minimum error variance assuming $\mathbf{x}_\mathrm{b}^i \sim N(\mathbf{x}_\mathrm{t}^i, \mathbf{B}^i)$ and $\mathbf{y}^i \sim N(h(\mathbf{x}_\mathrm{t}^i), \mathbf{R}^i)$; that is, the background and observation errors are Gaussian-distributed, unbiased estimates of the truth $\mathbf{x}_\mathrm{t}^i$, and their error covariances are accurately given by $\mathbf{B}^i$ and $\mathbf{R}^i$. It is also assumed that the observation and background errors are uncorrelated with one another. An analytical expression for the analysis that minimises Equation (1) as a first-order approximation is then

$$\mathbf{x}_\mathrm{a}^i = \mathbf{x}_\mathrm{b}^i + \mathbf{K}^i(\mathbf{y}^i - h(\mathbf{x}_\mathrm{b}^i)), \quad (2)$$

where $\mathbf{K}^i$ is the Kalman gain matrix given by a function of $\mathbf{B}^i$ and $\mathbf{R}^i$ and the observation operator linearised about the state, $\mathbf{H}^i$:

$$\mathbf{K}^i = \mathbf{B}^i(\mathbf{H}^i)^\mathrm{T}\left(\mathbf{H}^i\mathbf{B}^i(\mathbf{H}^i)^\mathrm{T} + \mathbf{R}^i\right)^{-1}. \quad (3)$$

The error in the analysis given by $\epsilon_\mathrm{a}^i = \mathbf{x}_\mathrm{a}^i - \mathbf{x}_\mathrm{t}^i$ has the following covariance matrix:

$$\mathbf{P}_\mathrm{a}^i = (\mathbf{I} - \mathbf{K}^i\mathbf{H}^i)\mathbf{B}^i; \quad (4)$$

see (Kalnay, 2003).

If biases are present in the background or observations, then the analysis given by Equation (2) will still be the state with the minimum error variance, as described by Equation (4), but the analysis will now be biased. It follows from Equation (2) that the bias in the analysis will be given by

$$\boldsymbol{\beta}_\mathrm{a}^i = \boldsymbol{\beta}_\mathrm{b}^i + \mathbf{K}^i(\boldsymbol{\beta}_\mathrm{y}^i - h(\boldsymbol{\beta}_\mathrm{b}^i)), \quad (5)$$

where $\boldsymbol{\beta}_\mathrm{b}^i$ and $\boldsymbol{\beta}_\mathrm{y}^i$ are the biases in the background and observations respectively. In the remainder of this article, we assume, for simplicity, that the observation operator is linear such that Equation (5) may be written as

$$\boldsymbol{\beta}_\mathrm{a}^i = (\mathbf{I} - \mathbf{K}^i\mathbf{H}^i)\boldsymbol{\beta}_\mathrm{b}^i + \mathbf{K}^i\boldsymbol{\beta}_\mathrm{y}^i. \quad (6)$$

From Equation (6), we see that if the observations are unbiased ($\boldsymbol{\beta}_\mathrm{y}^i = \mathbf{0}$) then the reduction in the bias in the analysis compared with the background depends on the weighting given to the observations ($\mathbf{K}$). In regions where there is little information in the observations, the bias in the analysis will remain close to that of the background.

The expected outer product of the error (EOPE) of the analysis, $E[(\mathbf{x}_\mathrm{a}^i - \mathbf{x}_\mathrm{t}^i)(\mathbf{x}_\mathrm{a}^i - \mathbf{x}_\mathrm{t}^i)^\mathrm{T}] = \mathbf{P}_\mathrm{a}^i + \boldsymbol{\beta}_\mathrm{a}^i(\boldsymbol{\beta}_\mathrm{a}^i)^\mathrm{T}$, is then

$$\begin{aligned}\mathrm{EOPE}_\mathrm{a}^i = {} & (\mathbf{I} - \mathbf{K}^i\mathbf{H}^i)\mathbf{B}^i \\ & + (\mathbf{I} - \mathbf{K}^i\mathbf{H}^i)\boldsymbol{\beta}_\mathrm{b}^i\boldsymbol{\beta}_\mathrm{b}^{i\,\mathrm{T}}(\mathbf{I} - \mathbf{K}^i\mathbf{H}^i)^\mathrm{T} \\ & + \mathbf{K}^i\boldsymbol{\beta}_\mathrm{y}^i\boldsymbol{\beta}_\mathrm{y}^{i\,\mathrm{T}}\mathbf{K}^{i\mathrm{T}} + (\mathbf{I} - \mathbf{K}^i\mathbf{H}^i)\boldsymbol{\beta}_\mathrm{b}^i\boldsymbol{\beta}_\mathrm{y}^{i\,\mathrm{T}}\mathbf{K}^{i\mathrm{T}} \\ & + \mathbf{K}^i\boldsymbol{\beta}_\mathrm{y}^i\boldsymbol{\beta}_\mathrm{b}^{i\,\mathrm{T}}(\mathbf{I} - \mathbf{K}^i\mathbf{H}^i)^\mathrm{T}. \end{aligned} \quad (7)$$

Note that the mean of the diagonal values of the EOPE matrix, $(1/N)trace(\mathrm{EOPE})$, gives the MSE.

The bias in the analysis will be propagated to become the bias in the background at the following assimilation cycle by the forecast model $\mathcal{M}$ and will include the bias in the model accumulated over the forecast, $\mathbf{b}^i$:

$$\boldsymbol{\beta}_\mathrm{b}^{i+1} = \mathcal{M}(\boldsymbol{\beta}_\mathrm{a}^i) + \mathbf{b}^i. \quad (8)$$

Similarly, the analysis error covariance will be propagated to become the background error covariance matrix at the following assimilation cycle by the linearised forecast model M and will include the error covariance of the model accumulated over the forecast, $\mathbf{Q}$:

$$\mathbf{B}^{i+1} = \mathbf{M}\mathbf{P}_\mathrm{a}^i\mathbf{M}^\mathrm{T} + \mathbf{Q}. \quad (9)$$

If the model error is truly a bias and deterministic then this will not contribute to **Q**. As such, for this study, we will not consider **Q** further.

2.1 | Explicit BC

If $\boldsymbol{\beta}_{\mathrm{b}}^{i}$ is known then this can be removed from the background before assimilation. The analysis bias is then given by the weighted observation bias only:

$$\boldsymbol{\beta}_{\mathrm{a}}^{\mathrm{BC},i} = \mathbf{K}^{i}\boldsymbol{\beta}_{\mathrm{y}}^{i}. \tag{10}$$

The BC superscript is used to label all vectors and matrices derived using the explicit BC. Thereafter, the bias in the background—see Equation (8)—will be

$$\boldsymbol{\beta}_{\mathrm{b}}^{\mathrm{BC},i+1} = \mathcal{M}(\mathbf{K}^{i}\boldsymbol{\beta}_{\mathrm{y}}^{i}) + \mathbf{b}^{i}, \tag{11}$$

which could continue to be removed at each assimilation time. The analysis error covariance is unchanged by the BC, and so is of the same form as Equation (4):

$$\mathbf{P}_{\mathrm{a}}^{\mathrm{BC},i} = \mathbf{P}_{\mathrm{a}}^{i} = (\mathbf{I} - \mathbf{K}^{i}\mathbf{H}^{i})\mathbf{B}^{i}. \tag{12}$$

The EOPE of the analysis in this case is given by

$$\mathrm{EOPE}_{\mathrm{a}}^{\mathrm{BC},i} = \mathbf{P}_{\mathrm{a}}^{\mathrm{BC},i} + \mathbf{K}^{i}\boldsymbol{\beta}_{\mathrm{y}}^{i}\boldsymbol{\beta}_{\mathrm{y}}^{i\,\mathrm{T}}(\mathbf{K}^{i})^{\mathrm{T}}. \tag{13}$$

Instead of removing the background bias in one step, a correction to the model could instead be applied at each time step of the model evolution between the current analysis time and the next. This may be advantageous in terms of the stability of the model and counteracting the effects of the nonlinearity of the model on the developing bias but does not impact the theory presented here.

2.2 | Covariance inflation

In the presence of a background bias, Dee and Da Silva (1998) showed that the analysis with the smallest MSE ($\frac{1}{N}\mathit{trace}(\mathbf{P}_{\mathrm{a}} + \boldsymbol{\beta}_{\mathrm{a}}(\boldsymbol{\beta}_{\mathrm{a}})^{\mathrm{T}})$) is given by assimilating the data using a background error covariance matrix inflated by the outer product of the background bias:

$$\tilde{\mathbf{B}}^{i} = \mathbf{B}^{i} + \boldsymbol{\beta}_{\mathrm{b}}^{i}(\boldsymbol{\beta}_{\mathrm{b}}^{i})\mathrm{T}. \tag{14}$$

The analytical expression for the analysis then has the same form as Equation (2) but with **K** replaced by

$$\tilde{\mathbf{K}}^{i} = \tilde{\mathbf{B}}^{i}(\mathbf{H}^{i})^{\mathrm{T}}(\mathbf{H}^{i}\tilde{\mathbf{B}}^{i}(\mathbf{H}^{i})^{\mathrm{T}} + \mathbf{R}^{i})^{-1}. \tag{15}$$

The modified Kalman gain matrix means less weight is given to the background and so the assimilation is given more freedom to fit to the observations. Inflating not only the variances but also the correlations means that the observations can correct biases over large regions and spread the correction to unobserved areas and variables. Inflation is a much gentler approach to correcting the bias, as only information on the magnitude of the bias is provided and not the sign.

In this case, the bias in the analysis is given by

$$\boldsymbol{\beta}_{\mathrm{a}}^{\mathrm{CI},i} = (\mathbf{I} - \tilde{\mathbf{K}}^{i}\mathbf{H}^{i})\boldsymbol{\beta}_{\mathrm{b}}^{i} + \tilde{\mathbf{K}}^{i}\boldsymbol{\beta}_{\mathrm{y}}^{i}. \tag{16}$$

The CI superscript is used to label all vectors and matrices derived using the CI. The CI means that more weight is given to the observations such that $(\mathbf{I} - \tilde{\mathbf{K}}\mathbf{H}) < (\mathbf{I} - \mathbf{K}\mathbf{H})$. Therefore, if the observations are unbiased, $\boldsymbol{\beta}_{\mathrm{a}}^{\mathrm{CI}} < \boldsymbol{\beta}_{\mathrm{a}}$. The bias reduction is largest when the inflation is greatest, which is when the background bias is largest. In the scalar case, the ratio between the bias in the analysis with CI and without (again assuming the observations are unbiased) is given by

$$\frac{\beta_{\mathrm{a}}^{\mathrm{CI}}}{\beta_{\mathrm{a}}} = \frac{\sigma_{\mathrm{y}}^{2} + \sigma_{b}^{2}}{\sigma_{\mathrm{y}}^{2} + \sigma_{\mathrm{b}}^{2} + \beta_{\mathrm{b}}^{2}}. \tag{17}$$

Therefore, from Equation (17), we also see that the bias reduction is also greatest when the observation and background error standard deviations are small compared with the bias; that is, the bias is significant compared with the random error.

If the observations are biased, $\boldsymbol{\beta}_{\mathrm{y}}^{i} \neq 0$, then the CI will also give more weight to the biased observations and spread this bias via the inflated background error correlations. Therefore, CI could be more susceptible to biased observations than explicit BC.

The analysis error covariance matrix when CI is applied is given by

$$\mathbf{P}_{\mathrm{a}}^{\mathrm{CI},i} = (\mathbf{I} - \tilde{\mathbf{K}}^{i}\mathbf{H}^{i})\tilde{\mathbf{B}}^{i} - (\mathbf{I} - \tilde{\mathbf{K}}^{i}\mathbf{H}^{i})\boldsymbol{\beta}_{\mathrm{b}}^{i}\boldsymbol{\beta}_{\mathrm{b}}^{i\mathrm{T}}(\mathbf{I} - \tilde{\mathbf{K}}^{i}\mathbf{H}^{i})^{\mathrm{T}}. \tag{18}$$

This includes a correction term to account for the fact that the true B matrix (i.e., the covariance of the random background errors only) is not used during the assimilation—see Eyre and Hilton (2013). The correction term is subtracted as the overestimation of the background error covariances will also lead to an overestimation of the analysis error covariances if evaluated using Equation (4). In the scalar case it is simple to show that $\mathbf{P}_{\mathrm{a}}^{\mathrm{CI}} > \mathbf{P}_{\mathrm{a}}$. The generalisation of this result to the multivariate case is discussed in Eyre and Hilton (2013).

The EOPE of the analysis is then

$$\begin{aligned}\mathrm{EOPE}_{\mathrm{a}}^{\mathrm{CI},i} = (\mathbf{I} - \tilde{\mathbf{K}}^{i}\mathbf{H}^{i})\tilde{\mathbf{B}}^{i} + \tilde{\mathbf{K}}^{i}\boldsymbol{\beta}_{\mathrm{y}}^{i}(\tilde{\mathbf{K}}^{i}\boldsymbol{\beta}_{\mathrm{y}}^{i})^{\mathrm{T}} \\ + (\mathbf{I} - \tilde{\mathbf{K}}^{i}\mathbf{H}^{i})\boldsymbol{\beta}_{\mathrm{b}}^{i}\boldsymbol{\beta}_{\mathrm{y}}^{i\,\mathrm{T}}\tilde{\mathbf{K}}^{i\mathrm{T}} \\ + \tilde{\mathbf{K}}^{i}\boldsymbol{\beta}_{\mathrm{y}}^{i}\boldsymbol{\beta}_{\mathrm{b}}^{i\,\mathrm{T}}(\mathbf{I} - \tilde{\mathbf{K}}^{i}\mathbf{H}^{i})^{\mathrm{T}}.\end{aligned} \tag{19}$$

If the observations are unbiased (i.e., $\boldsymbol{\beta}_{\mathrm{y}} = 0$) this will be consistent with the minimum MSE possible for assimilating the given data.

The smaller analysis bias when using CI will be propagated to become the bias in the background at the next assimilation time using Equation (8). Similarly, the larger analysis error covariance matrix using CI will be propagated to become the background error covariance matrix at the next assimilation time using Equation (9).

2.3 | Estimating the bias

In applying both the explicit BC and CI methods, knowledge of the bias in the background is needed. In practice, the background bias cannot be known precisely. This is in part due to the multifarious nature of the sources of the background bias making it a function of many different parameters causing it to vary in time and space. The background bias, however, can be estimated in regions of dense and *unbiased* observations (Laloyaux *et al.*, 2022).

A sample estimate of the background bias in the jth state variable may be given by

$$\hat{\beta}_{\mathrm{b},j} = \frac{1}{N_{S_j}} \sum_{k \in S_j} [y(k) - h(x_{\mathrm{b},j}(k))], \tag{20}$$

where $\mathbf{y}(S_j)$ is the subset of unbiased observations relevant to estimating the bias in the variable $\mathbf{x}_j$ and N_{S_j} is the size of this sample.

Let the error in the sample estimate of $\boldsymbol{\beta}_{\mathrm{b}}$ be given by

$$\boldsymbol{\epsilon} = \boldsymbol{\beta}_{\mathrm{b}} - \hat{\boldsymbol{\beta}}_{\mathrm{b}}. \tag{21}$$

The expectation of $\boldsymbol{\epsilon}$ is zero; that is, $\hat{\boldsymbol{\beta}}_{\mathrm{b}}$ is an unbiased estimate of the bias if the samples are independent (Lewis *et al.*, 2006). This means that if $\hat{\boldsymbol{\beta}}_{\mathrm{b}}$ was calculated repeatedly with different draws of the random variables $\mathbf{y}$ and $\mathbf{x}_{\mathrm{b}}$ then, on average, we would have a good representation of the background bias. In practice, though, the bias will only be estimated at most once for each assimilation time.

The variance of the error in the sample estimate for the jth variable is given by

$$var(\boldsymbol{\epsilon}_j) = \frac{\sigma^2_{\mathrm{d},j}}{N_{S_j}} \tag{22}$$

Lewis *et al.* (2006), where $\sigma^2_{\mathrm{d},j}$ is the error variance of the innovation given by $\mathbf{R} + \mathbf{HBH}^{\mathrm{T}}$ in the multivariate case. Therefore, the error in the sample estimate will increase as the variance in the observations and background error increases and the sample size N_{S_j} decreases. The dependence of the sample error on the observation and background error variances can be compared back to Equation (17), the ratio of the bias in the analysis when corrected using CI to no correction. We see that the conditions that allow for the potential of the CI to reduce the bias to be the greatest compared with not accounting for the bias (small error variance in the observations and background) is also when the error in the sample estimate of the bias should be its smallest. This is a clear advantage of the CI method, although the opposite is also true: when the bias should have the least of an effect it is also most difficult to estimate.

To increase the sample size and reduce the variance of the sample error, Equation(22), we can reduce the number of parameters used to model the background bias. For example, we may assume that the bias is constant over a given time period or spatial region, effectively making assumptions about the ergodicity and homogeneity of the background bias—see Bonavita and Laloyaux (2020) for a discussion of this in the context of numerical weather prediction. It is not straightforward to determine the best way to parametrise the background bias, meaning that there will always be a trade-off between the number of parameters (the model complexity for the bias) and the sampling noise. Simple assumptions of ergodicity and homogeneity may be particularly unsuitable in geophysical models where, for example, the domain can have complex boundary conditions, such as coastlines and model dynamics between different components of the Earth systems are coupled (e.g., atmosphere–land–sea). The parametrisation of model bias is, therefore, a good candidate for machine-learning tools, which may be expanded to learn nonlinear relationships, and has been the subject of previous studies Farchi *et al.* (2021); Bonavita and Laloyaux (2020); Bocquet *et al.* (2020); Brajard *et al.* (2020). Choosing how to parametrise the bias can also benefit from physical knowledge to ensure the BC does not disrupt balances within the model and to avoid unphysical instabilities, for example, Bonavita and Laloyaux (2020) pointed out the need to ensure that the learned corrections are vertically balanced. However, even with the most sophisticated machine learning algorithms the problems of sample size are still a challenge, and structural errors due to an oversimplification of how the bias varies remain.

The error in the estimate of the bias from a sample of innovations will have an impact on the explicit BC theory presented in Section 2.1. Owing to the error in the sample estimate of the background bias, BC will no longer completely remove the background bias contribution to the analysis bias—previously given by Equation (10). Instead, the bias in the background will now be

$$\hat{\boldsymbol{\beta}}_{\mathrm{b}}^{\mathrm{BC},i} = \boldsymbol{\epsilon}. \tag{23}$$

In the analysis, this will be reduced to (ignoring for now any possible observation bias)

$$\hat{\beta}_{\mathrm{a}}^{\mathrm{BC},i} = (\mathbf{I} - \mathbf{K}^i\mathbf{H}^i)\epsilon, \tag{24}$$

which will then be propagated to the next assimilation time as in Equation (8).

The uncertainty in the bias estimate from the innovation sample used to correct the background will increase the error standard deviation of the background, to become

$$\hat{\mathbf{B}} = \mathbf{B} + \hat{\mathbf{P}}, \tag{25}$$

where $\hat{\mathbf{P}}$ is the sample error covariance projected into state space given by

$$\hat{\mathbf{P}} = \boldsymbol{\Gamma}\mathbf{Z}\mathbf{D}\mathbf{Z}^{\mathrm{T}}\boldsymbol{\Gamma}^{\mathrm{T}}. \tag{26}$$

$\boldsymbol{\Gamma}$ is the mapping from the parameter space of the background bias to the state space, $\mathbf{Z}$ is the mapping from observation to parameter space, and $\mathbf{D}$ is the covariance of the innovation scaled by the size of the sample, as in Equation 22). For example, if the background bias is estimated from N observations that fully observe the state at each grid point and the bias is estimated for each state variable then $\hat{\mathbf{P}} = (1/N)(\mathbf{R} + \mathbf{B})$. If the bias estimate is parametrised at a much coarser resolution than the model grid then $\boldsymbol{\Gamma}\mathbf{Z}$ will have the effect of introducing larger length scales into $\hat{\mathbf{B}}$.

If the uncertainty due to the sample estimate is not accounted for then this will impact the analysis error covariance, and instead of Equation (12), the following will be true:

$$\hat{\mathbf{P}}_{\mathrm{a}}^{\mathrm{BC},i} = (\mathbf{I} - \mathbf{K}^i\mathbf{H}^i)\mathbf{B}^i + (\mathbf{I} - \mathbf{K}^i\mathbf{H}^i)\hat{\mathbf{P}}(\mathbf{I} - \mathbf{K}^i\mathbf{H}^i)^{\mathrm{T}}. \tag{27}$$

The EOPE of the BC method then taking into account sample error will be

$$\widehat{\mathrm{EOPE}}_{\mathrm{a}}^{\mathrm{BC},i} = \hat{\mathbf{P}}_{\mathrm{a}}^{\mathrm{BC},i} + (\mathbf{I} - \mathbf{K}^i\mathbf{H}^i)\epsilon\epsilon^{\mathrm{T}}(\mathbf{I} - \mathbf{K}^i\mathbf{H}^i)^{\mathrm{T}}. \tag{28}$$

We could then propose a modification to the BC method that takes into account the uncertainty in the bias estimate. This could be achieved in a way that again does not require changes to the data assimilation algorithm by inflating the B matrix to include the sample error uncertainty as in Equation (25) and will be discussed in the numerical experiments in Section 3.

As the bias estimate is not used to directly correct the state in the application of the CI method, it will not affect the theory presented in Section 2.2. This may have the benefit of allowing CI to be more robust to the sample errors than BC. However, it will no longer be true that the CI method (when observations are unbiased) provides the minimum MSE analysis.

To increase the sample size and overcome the restrictions of the available observing systems, aspects of the model bias could also be learnt from the analysis increments, (Bonavita & Laloyaux, 2020). However, the $\boldsymbol{\beta}_{\mathrm{b}}$ estimated from analysis increments will still be limited by the availability of unbiased observations. The bias estimated will also be subject to the specified B matrix and the accuracy of the multivariate correlations and biases in the observation (Laloyaux *et al.*, 2022). For these reasons, estimating the uncertainty in the bias estimate derived from analysis increments, to get an equivalent of Equation (26), is more challenging.

Lastly, we comment on WC-4DVar, which aims to estimate and correct the model bias online given a first guess of the model bias and an estimate of the error covariance of that first guess. This is advantageous over explicit BC, in that it is acknowledged that the estimated bias has some error. By using a window of observations, WC4D-Var will also be more likely to find a BC that does alter the stability of the model. However, WC4D-Var is still reliant on the presence of unbiased observations and is restricted by the assumptions made about the structure of the model bias (Laloyaux *et al.*, 2020). WC4D-Var also has a disadvantage in that it requires the data assimilation algorithm to be modified and the size of the state to be optimised to be increased, making the assimilation problem more complex and more nonlinear.

In the next section, we illustrate how explicit BC and CI are sensitive to the estimate of the background bias, including the effects of sample noise, structural errors, and smoothing the bias spatially.

3 | NUMERICAL EXPERIMENTS

3.1 | Idealised data assimilation system

To illustrate the ability of the explicit BC method and the CI method to give an unbiased analysis we set up an idealised linear system in which, without any methods to control the bias, the background error covariance and background bias remain constant as the assimilation system is cycled. That is, the growth of the errors due to model evolution is perfectly counteracted by the contraction of the errors that occurs at each assimilation time step; that is, $\boldsymbol{\beta}_{\mathrm{b}}^{i+1} = \boldsymbol{\beta}_{\mathrm{b}}^{i}$ and $trace(\mathbf{B}^{i+1}) = trace(\mathbf{B}^{i})$.

For an optimal system where $\mathbf{K}$ uses the correct covariance matrices and $\mathbf{Q} = 0$, combining Equations 4 and 9 finds that for $trace(\mathbf{B})$ to remain constant $\mathbf{M}$ would satisfy

$$\mathbf{M}^{\mathrm{T}}\mathbf{M} = (\mathbf{I} - \mathbf{K}\mathbf{H})^{-1}. \tag{29}$$

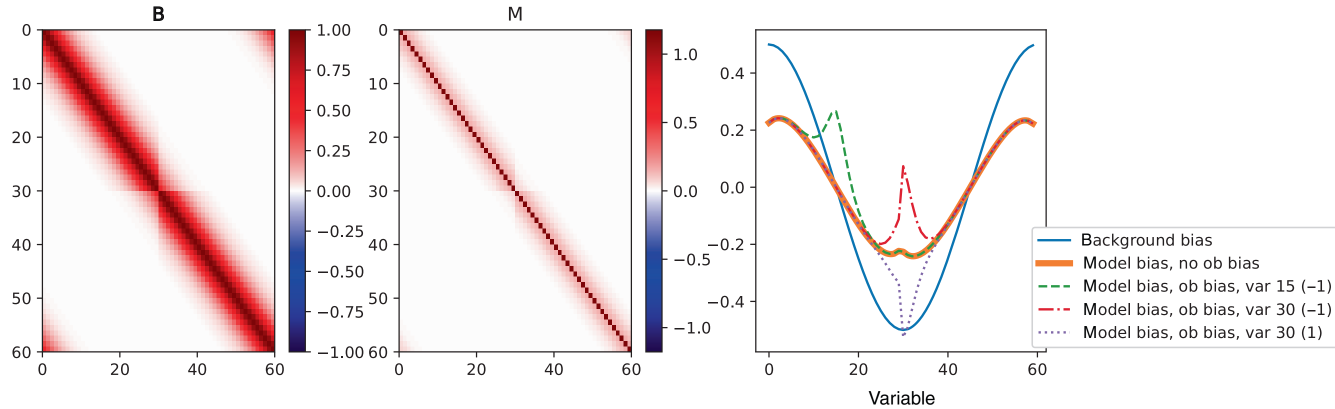

FIGURE 1 Experiment set-up. Given **B** matrix (left) and resulting linear model **M** (middle). On the right is the given background bias (blue) and resulting model bias when observations are unbiased (orange), one instrument measuring variable 15 has a bias of −1 (dashed green), one instrument measuring variable 30 has a bias of −1 (dash-dotted red), and one instrument measuring variable 30 has a bias of 1 (dotted purple). [Colour figure can be viewed at wileyonlinelibrary.com]

For the background bias $\boldsymbol{\beta}_{\rm b}$ to remain constant, combining Equations 6 and 8 finds that the model bias must satisfy

$$\mathbf{b} = [\mathbf{I} - \mathbf{M}(\mathbf{I} - \mathbf{KH})]\boldsymbol{\beta}_{\rm b} - \mathbf{MK}\boldsymbol{\beta}_{\rm y}. \quad (30)$$

In the following experiments the state is given by a variable on a periodic domain discretised into 60 grid points. The **B** matrix is given by a circulant matrix with the correlation between two points separated in distance by r_k given by the second-order autoregressive function

$$c_k = (1 + r_k/L)\exp(-r_k/L) \quad (31)$$

with length-scale $L = 2$ and an error variance of 1 for each of the 60 variables. The coupling between the two halves of the domain is weakened by multiplying the covariances between the two halves by 0.5, illustrated in the left-hand panel of Figure 1.

The observations directly observe the state variables, such that $\mathbf{H} = \mathbf{I}$. To compensate for this dense observing network, which would be unlikely in most applications, the error variance is set to 5 for each observation. The observation errors are uncorrelated, so that $\mathbf{R} = 5 \times \mathbf{I}$.

Given these prescribed **B**, **R**, and **H** matrices we then compute $\mathbf{M}^{\rm T}\mathbf{M}$ using Equation (29). To define the linear model **M** we apply eigendecomposition such that $\mathbf{U}\boldsymbol{\Lambda}\mathbf{U}^{\rm T} = \mathbf{M}^{\rm T}\mathbf{M}$ and choose $\mathbf{M} = \mathbf{U}\boldsymbol{\Lambda}^{1/2}\mathbf{U}^{\rm T}$. This symmetric **M** is illustrated in the middle panel of Figure 1. The weak coupling in the background error covariances means that the model is also weakly coupled between the two halves of the domain. Note that there are many other **M** matrices that would be consistent with Equations (29); for example, $\mathbf{V}\boldsymbol{\Lambda}^{1/2}\mathbf{U}^{\rm T}$, where **V** is any orthonormal matrix.

The background bias, which is constant in time, is defined for the jth grid point as

$$\beta_{{\rm b},j} = \frac{1}{2}\cos(2\pi j/60). \quad (32)$$

This is shown by the blue line in the right-hand panel of Figure 1. The magnitude of the background bias peaks at the edges of the two halves of the domain. This could be consistent with a source of model bias coming from systematic error in the coupling of the two subdomains. The maximum magnitude of the background bias, 0.5, is half the background error standard deviation.

In the following experiments, we consider four cases for the observation biases: (a) no biases are present in the observations; (b) one instrument measuring variable 15 (where the background bias is zero) has a bias of −1; (c) one instrument measuring variable 30 (where the background bias is −0.5) has a bias of −1; and (d) one instrument measuring variable 30 has a bias of +1. The relatively large observation bias (compared with the background bias) was chosen to emphasise its impact in the following experiments; however, it is still much less than the observation error standard deviation of $\sqrt{5}$.

To maintain this background bias with the given **M**, **B**, **R**, and **H**, the model bias is given by Equation (30). In the first case, no observation biases, the model bias is shown by the orange line in Figure 1. The weak coupling means that the model bias is locally decreased at the edge of the subdomain as less information from the observations can constrain this region and so the model bias needed to maintain the background bias is less. When the observations are biased, this affects the model bias needed to maintain the background bias. When the observation bias increases the mean innovation (as is the case

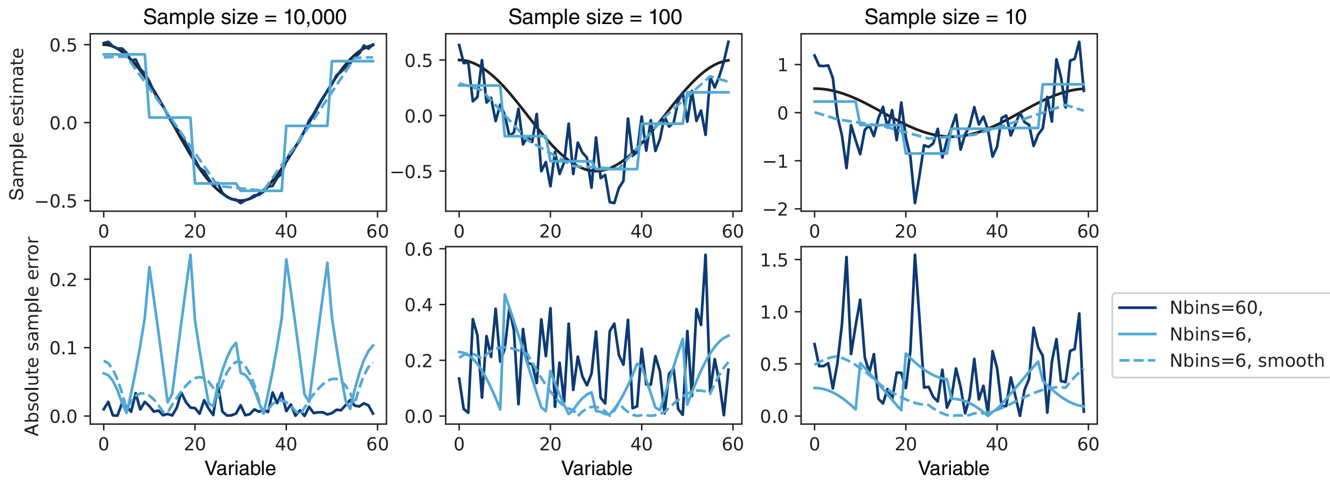

FIGURE 2 Top: Sample approximations to the true initial background bias (black line) for sample sizes of 10,000 (left), 100 (middle), and 10 (right). The intensity of the colour indicates the spatial averaging of the sample estimate (see legend). Bottom: Absolute sample error. [Colour figure can be viewed at wileyonlinelibrary.com]

when the observation bias is negative; green dashed and red dash-dotted lines), a smaller model bias is needed in the region of the biased observation compared with when the observations are unbiased. When the observation bias decreases the mean innovation (as is the case when the observation bias is positive; purple dotted line), a larger magnitude of the model bias is needed in this region. This response of the model bias to the observation bias is very contrived and not expected in practice but provides a clear baseline of a constant background bias across the different experiments.

3.2 | Sample estimates of the background bias

The background bias is estimated from a sample of innovations as in Equation (20), assuming direct observations, where the kth sample for the ith assimilation cycle is given by

$$\mathbf{d}_i^{(k)} = \boldsymbol{\eta}_{\mathrm{y}}^{(k)} - \boldsymbol{\eta}_{\mathrm{b},i}^{(k)}, \tag{33}$$

with $\boldsymbol{\eta}_{\mathrm{y}}^{(k)} \sim N(\boldsymbol{\beta}_{\mathrm{y}}, \mathbf{R})$ and $\boldsymbol{\eta}_{\mathrm{b},i}^{(k)} \sim N(\boldsymbol{\beta}_{\mathrm{b},i}, \mathbf{B}_i)$. Note, we only need to draw samples of the errors as the underlying truth will cancel when taking the difference in Equation (33).

In the following experiments, the background bias is estimated from a sample of 10,000, 100, and 10 innovations at each grid point. In practice, these sample sizes are unrealistically large. The choice of 10,000 is to allow for the performance of the schemes to be compared when the sampling error is negligible. The sample size of 100 and 10 may potentially be obtained from a time series of observations, with the assumption that the background bias is sufficiently constant over the sample.

Even if the model bias is constant in time, as we have imposed in our system, the background bias will change in time depending on how it is being corrected. To remove this complication from the interpretation of the results we draw a new sample of the innovations, Equation (33), at each time so that only the effect of sampling error is seen and not the added complexity of assuming the bias does not change in time.

As discussed in Section 2, to reduce the effect of the sampling error it is common to parametrise the bias. In the following, estimates of the bias for each grid box are compared with estimating the bias as a constant over 10 grid boxes (reducing the number of parameters from 60 to 6 and increasing the sample size for each bin 10 times).

The effect of the sample noise in estimating the initial background bias for each of these assumptions is shown in Figure 2 when the observations are unbiased. With a sample size of 10,000 (left-hand panels) and estimating the bias for every grid point, we see that we have a near-perfect estimate (the error in the estimate is about 5% of the magnitude of the maximum bias of 0.5). This allows us to see the effect of the binning of the data. With only six bins the variability in the bias is no longer captured and the error in the sample estimate is increased to about 50% of the maximum magnitude of the bias, particularly at the edge of the bins.

As the sample size is reduced, the larger bin sizes become more beneficial for reducing the error in the estimate of the bias. When the sample size is 10, without the binning of the data the error in the estimate is about 200% of the magnitude of the bias, reduced to 100% the magnitude of the bias when the estimate is coarsened.

To remove the discontinuous effect of the large bin size, additional smoothing can be applied so that an estimate of the bias is given for each grid box as a weighted combination of the estimate from the two nearest values depending on the distance from the centre of the bins. The effect of this is shown in Figure 2 by the dashed lines. The additional smoothing reduces the sampling error in each case.

If an instrument used to estimate the background bias from Equation (33) itself has a bias, then this will be included in the estimate of the background bias. If only one instrument has a bias then the impact on the estimate of the background bias will be negligible when the estimate is coarsened or smoothed.

4 | RESULTS

4.1 | Accounting for bias when the bias is known perfectly

For the experimental set-up described in Section 3, we first compare the performance of the explicit BC and CI when the background bias is perfectly known as a baseline for the experiments when the bias is not known exactly. The left-hand panels in Figure 3 show the background statistics, and the right-hand panels show the analysis statistics for the case when there are no biases present in the observations as a function of 10 assimilation cycles.

Without any BC (the control, black line) the bias in the analysis is reduced to an average value of 0.08 compared with 0.31 in the background (a reduction of approximately 70%), whereas the mean error variance is reduced from 1 in the background to 0.382 in the analysis (a reduction of approximately 60%).

At the initial cycle, the CI (red lines) background bias is the same as in the control and the background error variances are also the same. After, the initial cycle, however, the CI background bias reduces but the error variance increases; however, overall, the MSE of the CI background is reduced compared with the control. On the other hand, as the bias is perfectly corrected in the BC (blue lines) background, the background bias remains constantly zero as the assimilation cycles progress and the BC background MSE is constantly equal to one. After assimilation, we see that CI reduces the analysis bias by about 50% compared with the control and increases the analysis error variances by about 0.4%. So, overall, the MSE is reduced by 1%. In contrast, the BC completely removes the bias and leaves the analysis error variances unchanged, reducing the MSE by 2%.

For comparison, we also show the case when only the variances are inflated and no change is made to the correlations in the **B** matrix (VI, green lines). This is a simplification of the CI method. Compared with CI, this has a much more limited ability to reduce the analysis bias and has a much more dramatic impact on inflating the analysis error variances as the assimilation is cycled, so that the analysis MSE is overall much worse than not accounting for the bias at all.

The importance of inflating the correlations as well as the variances is further illustrated in Figure 4, in which the effect of including the outer product of the bias on the covariance structure of **B** and subsequently the sensitivity of the analysis to the observations given by $\tilde{\mathbf{K}}$ is shown. In the left-hand panel, the structure of **K** (no CI) is shown. We see that the sensitivities on the diagonal (the so-called self-sensitivities) are about 0.2. The off-diagonal elements (the cross-sensitivities) then show how the information from the observations is spread to the neighbouring points, with reduced spreading at the edge of the subdomains. The CI causes large changes in the structure of the inflated **B** (middle panel of Figure 4, cf. Figure 1), giving both positive and negative correlations at much larger distances than without inflation and increasing the coupling between the two subdomains. The change in the **B** matrix has the effect of increasing the self-sensitivities and cross-sensitivities in the regions where the bias is of the same sign but giving negative cross-sensitives between the regions where the bias has a different sign (as seen in $\tilde{\mathbf{K}} - \mathbf{K}$ in the right-hand panel of Figure 4). The change to the **K** matrix that the CI causes allows a single observation to reduce the bias across the domain. However, if the inflation is not applied correctly then this could have a large impact on the balances implied by the B matrix.

Experiments in which one instrument contained a bias, as described in Section 3, were also performed in the case when the background bias was perfectly known and accounted for with the two methods and compared with the control when no attempt is made to account for the bias. The effect of the observation bias on the analysis mean and MSE at the 10th assimilation cycle is summarised in Table 1. We see that the sensitivity of the different methods to the observation bias depends on how the bias in the observations relates to the bias in the background. If the observation bias reduces the mean innovation (as is the case when the observation of variable 30 has a positive bias) then the presence of the observation bias generally has a smaller negative impact than if the observation bias increases the mean innovation. However, as anticipated, the CI method is the most sensitive to the presence of an observation bias, particularly in terms of the analysis bias.

The effect of the observation bias on the analysis bias with the different methods is even more evident in Figure 5, in which the analysis bias is plotted as a function of the variables for the 10th assimilation cycle. We see how in each case the analysis bias is pulled towards

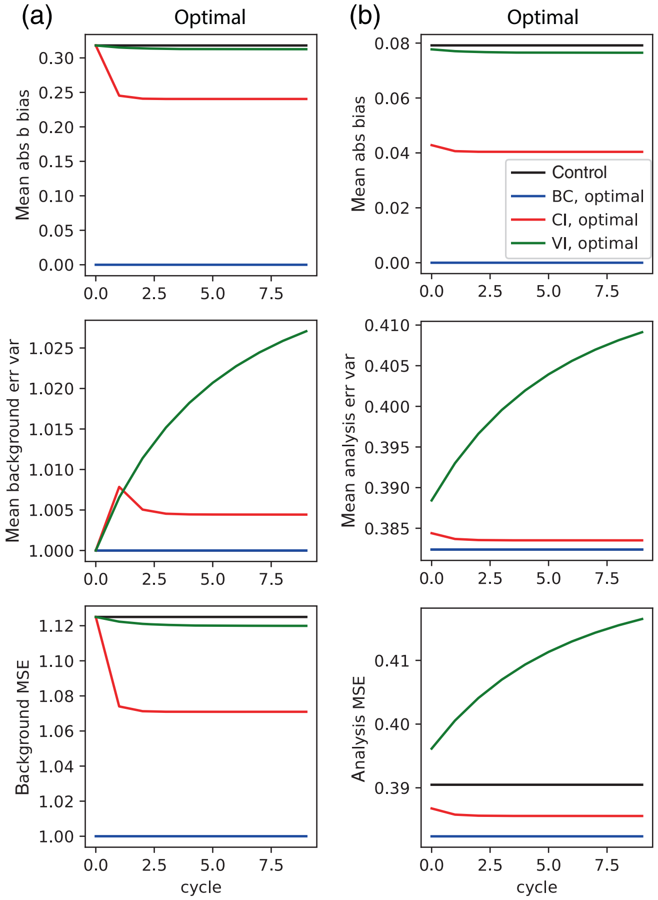

FIGURE 3 The mean absolute bias (top), mean error variance (middle) and mean-square error (MSE; bottom) for the background (left) and analysis (right) as a function of the assimilation cycle. The blue and red lines are when bias correction (BC) and covariance inflation (CI) are applied respectively and the bias is known *exactly*. The green line is when only the variances are inflated (VI) as an approximation to the CI method. This can be compared with the control when no attempt is made to correct the bias (black line). Note the control mean error variance cannot be seen as it lies directly under BC line. [Colour figure can be viewed at wileyonlinelibrary.com]

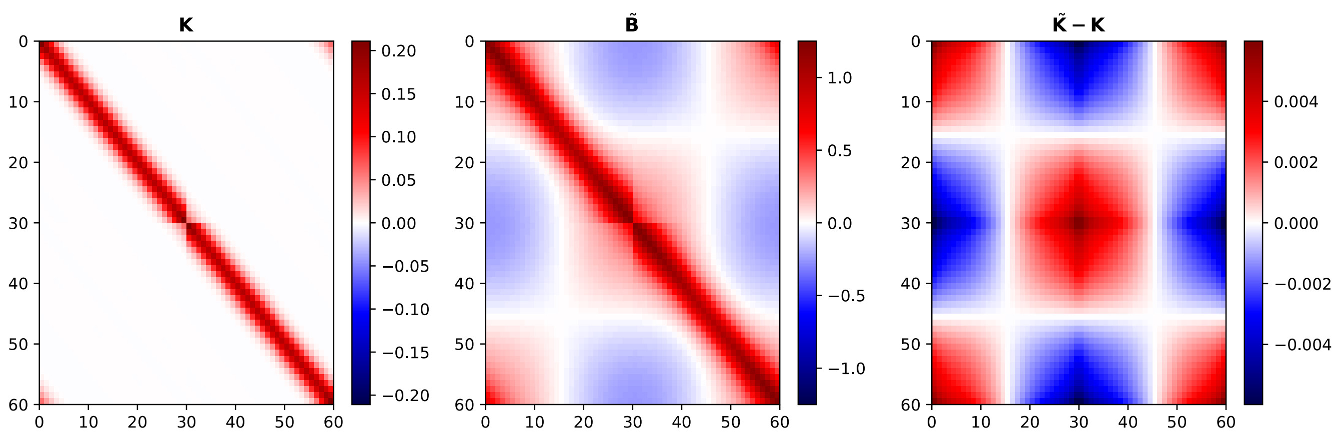

FIGURE 4 Left: the Kalman gain matrix, Equation (3); middle: the inflated background error covariance matrix, Equation (14), at the initial time; right: the difference between the Kalman gain with inflation, Equation (15), and without inflation. [Colour figure can be viewed at wileyonlinelibrary.com]

the observation bias. When the observation bias is in the instrument observing variable 15 (where the background bias is zero), we see that locally the analysis bias is similar for all three methods. When the observation bias is −1 in the instrument observing variable 30 (where the background bias is −0.5), we see that locally the CI method has a larger analysis bias than the BC method, but both have a smaller bias than the control. When the observation bias is 1 in the instrument observing variable 30 (where the background bias is −0.5), we see that locally the BC method has a marginally larger analysis bias than the CI method, but both have a larger bias than the control. It is not obvious from these plots that the effect of the observation bias is spread further with the CI method.

TABLE 1 Mean analysis bias, β^a, and MSE after 10 assimilation cycles for experiments with different observation biases, as described in Section 3.

	Control		BC		CI	
Ob bias (variable)	β^a	**MSE**	β^a	**MSE**	β^a	**MSE**
None	0.080	0.391	0	0.382	0.04	0.386
−1 (15)	0.090 (↑12.5%)	0.392 (↑0.25%)	0.015	0.382	0.052 (↑30%)	0.387 (↑0.3%)
−1 (30)	0.090 (↑12.5%)	0.395 (↑1%)	0.015	0.382	0.055 (↑37.5%)	0.389 (↑0.8%)
1 (30)	0.070 (↓12.5%)	0.389 (↓0.5%)	0.012	0.382	0.035 (↓12.5%)	0.385 (↓0.3%)

Note: The percentage change in the statistic compared with when the observations are unbiased is given in parentheses. BC: bias correction; CI: covariance inflation; MSE: mean-square error.

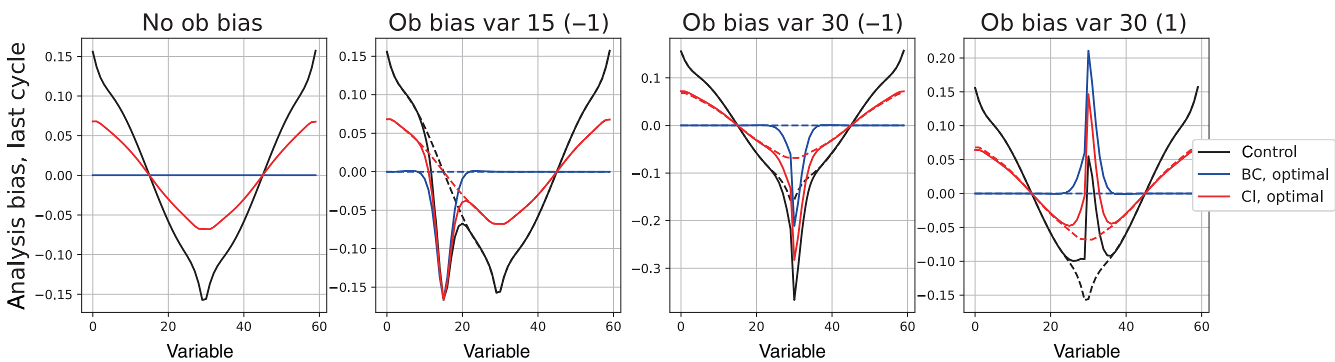

FIGURE 5 Analysis bias as a function of variable for the 10th assimilation cycle for when the background bias is unaccounted for (black) and accounted for using bias correction (BC; blue) and covariance inflation (CI; red). The different panels from left to right are for when the observations are unbiased, observation of variable 15 has a bias of −1, observation of variable 30 has a bias of −1, and observation of variable 30 has a bias of 1. The dashed lines are the analysis bias when the observations are unbiased. [Colour figure can be viewed at wileyonlinelibrary.com]

4.2 | Accounting for background bias when the bias is not known perfectly

Next, we look at the effect of the sampling error in the estimate of the background bias on the performance of the two methods when the observations are unbiased. The assimilation experiments are cycled in time with the two different methods for bias treatment (BC, CI) when the background bias is estimated from a sample of 10,000, 100, and 10 innovations at each grid point (see Section 3.2).

The results from performing 10 assimilation cycles are shown in Figure 6. When the sample size is large (first column) and the bias is estimated for every variable (dark lines) we see that the sampling noise has a limited impact on the effectiveness of the BC and CI methods. Therefore, the analysis statistics are very similar to when the bias was known exactly (cf. Figure 3) and so the BC method still outperforms the CI method.

When the sample size is large but the bias estimate is coarsened by decreasing the bins (light solid lines), the performance of both BC and CI deteriorates and results in an MSE that is worse after a couple of assimilation cycles than not attempting to correct for the bias at all. However, the CI method is more robust and performs better than the BC method. The bias for the BC method with coarsening increases rapidly with each cycle as the errors in performing the BC are propagated and make the bias estimation in the next cycle more difficult. With additional smoothing (light dashed lines) the performance of both BC and CI is again close to optimal.

As the sample size is reduced both BC and CI degrade when estimating the bias at every grid point. But again the CI method seems to be more robust, with the analysis bias using the CI method remaining smaller than the control when the sample size is 100 and similar to the control when the sample size is 10. In both cases, the analysis bias of the BC method is larger than the control. However, if the bin width is increased and additional smoothing is applied (dashed lines) then the performance of the two schemes is improved and the MSE is reduced again compared with not accounting for the bias.

Figure 7 shows the analysis bias as a function of the state variable for the 10th assimilation cycle. It can be seen how the sensitivity of the BC method can be explained

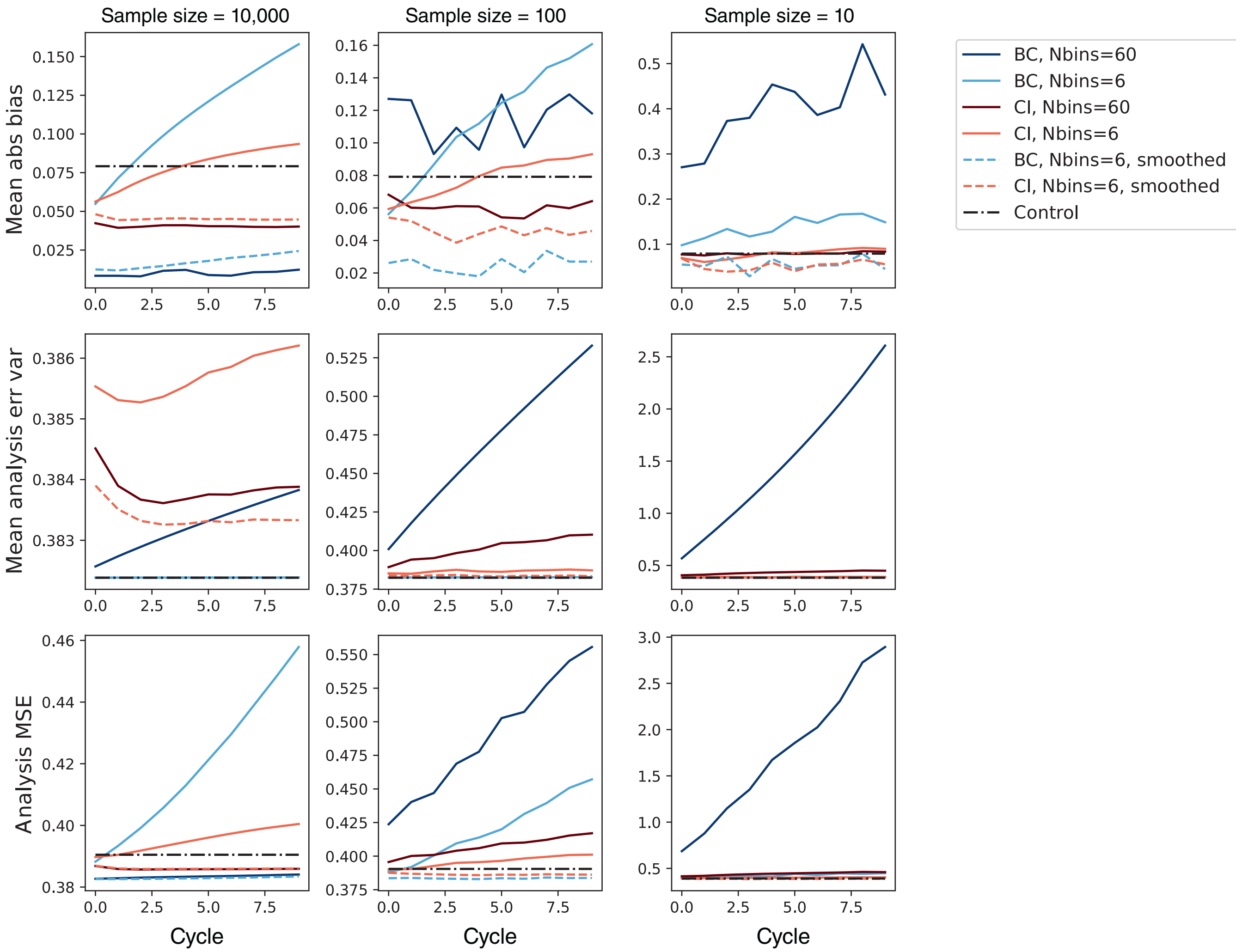

FIGURE 6 Mean absolute analysis bias (top row), mean analysis error variance (middle row), and analysis mean-square error (MSE; bottom row) as a function of the assimilation cycle when the background bias is estimated. In each column, the bias is estimated from a sample of innovations using Equation (20) with a sample size of 10,000 (left), 100 (middle), and 10 (right) with different numbers of bins. The background bias is then accounted for using bias correction (BC; blue lines) and covariance inflation (CI; red lines). The darker lines are when 60 bins are used, lighter lines are when six bins are used, and the dashed lines are when six bins are used with additional smoothing, as illustrated in Figure 2. In each panel, the black dashed line is the value achieved when the bias is not accounted for (i.e., the control in Figure 3). [Colour figure can be viewed at wileyonlinelibrary.com]

by the heterogeneity in the bias that is caused by the noise in the sample estimate. Both the CI and BC analysis biases are distributed about the optimal values given in the first panel (cf. Figure 5). However, the BC estimates suffer more from the sample noise; so, although centred on zero, they have much greater variability. The noise in the analysis will then propagate through to the forecast and can be expected to increase instabilities and decrease forecast skill.

Within these experiments, the differences between the different methods caused by the errors in the bias estimate tend to be greater than the differences caused by the presence of observation bias (cf. Table 1 and Figure 5).

The experiments were designed such that the domain was split in two with the two halves weakly coupled. This was done so that the change in the covariance structure caused by the inflation (cf. Figure 4) would reduce this property of the system. Within the experiments shown it is difficult to see any impact of this experimental design; however, experiments were also performed with differing background bias structures and differing coupling strengths between the two domains. Similar overall conclusions in terms of the two methods' sensitivity to the sample noise in the bias estimate can be drawn. From these experiments, however, it was additionally noticed that the bias in the analysis is more sensitive to error in

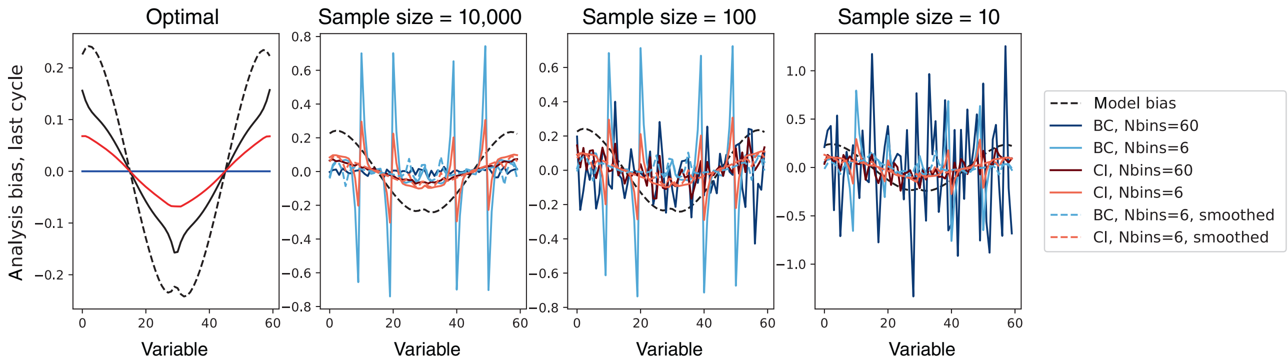

FIGURE 7 Analysis bias as a function of the state variable for the 10th cycle. Bias correction (BC; blue lines) and covariance inflation (CI; red lines) are performed when the bias is known exactly (first column, compared with the black line when not accounting for the bias), and estimated from a sample size of 10,000 (second column) and 100 (third column), and 10 (last column) with different numbers of bins (see legend). In each panel, the black dashed line shows the model error accumulated over each cycle. [Colour figure can be viewed at wileyonlinelibrary.com]

the background bias estimate as the assimilation is cycled in regions where the model bias is relatively small and at the interface of the subdomains when the coupling is weakened. Again, these sensitivities are greater for the BC method than the CI method.

5 | SUMMARY AND CONCLUSIONS

The aim of this short study was to provide insight on the relative advantages and disadvantages of two simple methods for accounting for background bias, namely explicit BC and CI. Each method relies on having an estimate of the background bias. When the background bias is well known BC outperforms CI, as it is able to remove the bias in the assimilation system completely and does not increase the analysis error covariances. However, in practice, the background bias must be inferred from a dataset of unbiased observations; and owing to the lack of observations and knowledge of how the bias changes spatially and temporally, the estimate of the bias will always be subject to error. Options for reducing the sample error include parametrising the bias so that it can be described by fewer variables than the model grid. Choosing the correct parameters is itself a challenge, and choosing too few could result in too coarse a representation of the background bias; we refer to this as a structural error within the bias estimate. Parametrising the bias is an obvious application for machine-learning techniques, but even with the most sophisticated techniques some uncertainty in the bias estimate will remain. Given this fact, this study showed that CI proved to be much more robust to errors in the bias estimate than the BC method, both in terms of sample noise and structural errors in the bias estimate.

This advantage of the CI method arises from its gentler approach to correcting the bias, allowing the observations to have greater freedom to correct for the background bias. In addition, the resulting increase in the analysis uncertainty has the benefit of acknowledging the presence of the underlying bias, whereas the BC method imposes a strict removal without any acknowledgement of the process. It was also shown that inflating the background error variances alone is not useful for reducing the background bias; therefore, the alteration of the covariance structure is crucial to the success of CI method. Although only experiments with a fully observed system were performed, the correlations would be even more essential when the system is only sparsely observed.

The effect of the sensitivity of the BC method to errors in the bias estimate was shown most evidently in the spatial plots of the analysis bias (see Figure 7). Here, it was clear that the noise in the analysis caused by errors in the bias estimate with the BC method are magnified as the assimilation system is cycled. Smoothing the bias estimate is therefore essential for the BC method. When the bias is parametrised in terms of spatial regions, then applying a smoothing algorithm is straightforward; however, for more complex parametrisation schemes (e.g., that might arise from machine learning), smoothing may be more difficult to implement, and so the application of machine learning should be done with this in mind.

For both methods, it is assumed in theory that the observations are unbiased. Experiments were performed to understand how a bias in an instrument observing a single variable might impact the analysis when the background bias is accounted for by the two methods. It was shown that the CI method is much more sensitive to the presence of an observation bias; but, depending on how the observation bias affects the mean innovation bias, the analysis bias in the vicinity of the biased observation could be largest with either the CI method, BC method, or not accounting for background bias at all (see Figure 5). The differences between the methods were illustrated for the case when observations were available of every grid point. However, it can be anticipated that the problem of observation biases would be greater when the observations are much sparser, such as with infrequent profiler observations available in the ocean.

The inadequacies of these simple approaches to accounting for background bias are overcome to a degree by WC4D-Var. The approach of WC4D-Var is to specify a first guess for the model bias normally accumulated over one time step and to then model the uncertainty in this with an error covariance matrix $\mathbf{Q}$. The estimate of the model bias is then updated given observations over a time window. The correlation structure in $\mathbf{Q}$ can be used to ensure that the updates to the bias estimate are smooth, and by taking a window of observations this will also help to mitigate instabilities being introduced that will be magnified as the model is propagated. However, WC4D-Var is still reliant on having many unbiased observations, and the specification of $\mathbf{Q}$ is non-trivial (Laloyaux *et al.*, 2020). Also, for many applications, this approach is simply not an option, due to the added complexities of the algorithm.

The application of the BC method with an inflated background error covariance matrix to account for the sampling error in the estimate of the background bias was also explored. Like WC4D-Var, this enhances the ability of the observations to make corrections to the BC applied. However, in our experiments (not shown), this was not found to be especially beneficial and was unable to counteract the noise already introduced by the BC.

These results were all illustrated in a univariate linear model, designed such that without BC the background error covariance matrix and background bias were static with successive assimilation cycles. This meant that the background bias to correct was clearly defined, which would not be the case if the model error also had a random component. This choice of model allowed for easy comparison between the different methods, removing the complexity of nonlinear effects on the analysis bias. However, the simplicity of this model has limited some of the conclusions that can be drawn. In future work, the impact of the different methods of BC on the stability of the dynamics will be studied in a model in which balances should be preserved during the assimilation. A multivariate model will also allow for a comparison of the BC methods when the bias can only be estimated for parts of the system due to the incomplete coverage of unbiased observations.

ACKNOWLEDGMENTS

I would like to thank Ross Bannister and Amos Lawless for useful discussion and feedback on the manuscript. This study was funded as part of NERC's support of the National Centre for Earth Observation, contract number PR140015.

DATA AVAILABILITY STATEMENT

The data that support the findings of this study are available from the corresponding author upon reasonable request.

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How to cite this article: Fowler, A.M. (2024) On the robustness of methods to account for background bias in data assimilation to uncertainties in the bias estimates. *Quarterly Journal of the Royal Meteorological Society*, 1–15. Available from: https://doi.org/10.1002/qj.4790