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Towards robust inversions: Parametric weighting of high-resolution TROPOMI observations for global methane emission estimates with TMVar (TM5-MP/4DVAR)

Author comments to RC1
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We would like to thank both referees for their constructive comments and corrections that helped to improve our manuscript. Hereby, we provide answers and comments on each of the points raised by the referees. Each comment of the reviewers is numbered and quoted in a gray box, followed by our replies and quoted text in a yellow box.

Anonymous Referee #1

(1) Line 46: The problem isn't just for variational inversions, it affects analytical versions too.

We changed the sentence to:

> However, in both analytical and variational inversions...

(2) Line 52: "...do not explicitly address local sampling density". That is not quite true when super-observations are used including error correlation for the individual observations, as shown by Chen et al. (2023).

We included the following sentences:

> Super-observations can provide an alternative by aggregating individual observations and accounting for their error correlations, thereby partly addressing local sampling density (Miyazaki et al., 2012; Chen et al., 2023; Nüß et al., 2025; Rijsdijk et al., 2025). This is limited to the observations contributing to each super-observation, and aggregation inevitably reduces the spatial and temporal detail retained from the original observation.

(3) Line 98: "...which are assumed to be uncorrelated". This is indeed standard practice but it is largely the problem you are trying to indirectly solve using density-based weighting. In fact, couldn't one argue that including spatial error correlation in the observational error covariance matrix is a more objective way to solve the uneven density problem?

The sentence has been extended for clarity:

> This error term includes instrument, representativeness, and model representation errors, which are often assumed to be uncorrelated. However, spatial correlations may exist, particularly among nearby satellite observations, and neglecting them can lead to an overestimation of the effective observational information they provide.

(4) Lines 111–112: "non-linearity of H... analytical solution is computationally unfeasible." That is definitely not true for methane unless one wants to invoke nonlinearity due to OH coupling on decadal scales, but that's not what this paper is about. The Harvard group has published a large number of papers on analytical inversions of methane, several of which are cited here, and this is implemented in the Integrated Methane Inversion (IMI; Varon et al., 2022, https://doi.org/10.5194/gmd-15-5787-2022) that a number of groups use. And the analytical inversion solves the problem with variational inversions raised on lines 119–122.

We agree that the nonlinearity of **H** alone does not forbid an analytical inversion. We have revised the text to clarify that our motivation for using a variational approach is the computational cost associated with high-dimensional inversion problems, rather than the nonlinearity of the forward model itself.

> For high-dimensional inversion problems, explicitly constructing and solving the corresponding analytical inverse problem can become computationally expensive. This is particularly relevant for high-resolution global inversions with large numbers of state variables and observations. Therefore, we apply a variational approach, in which the cost function J is minimized iteratively using a gradient-based optimization algorithm.

(5) Line 140, and elsewhere in the paper: I think it should be stated that observational error correlation is the theoretical best way to deal with differences in dataset density. I get the point that keeping R diagonal makes for easier inversion.

We agreed, and now it is mentioned in both the Introduction and Methodology sections.

> **Section 1. Introduction**
> Explicitly accounting for spatial error correlations would directly address this issue, but its implementation can be computationally demanding for large observational datasets.
>
> **Section 2.3. Regularization Factor**
> Explicitly representing spatial error correlations in the observational error covariance matrix would provide a more direct statistical treatment of this issue, provided that the correlation structure can be adequately characterized. However, constructing and handling a non-diagonal covariance matrix for large satellite datasets can substantially increase the computational cost of the inversion.

(6) Lines 157–159: fit to the chi-square distribution is also used for relative weighting of the prior and observation terms of the cost function through gamma, and in particular that's what is done in Lu et al., 2021 cited here. And there is no reason to expect gamma to be a "universally optimal constant factor" considering that it is intended to palliate for missing observational error correlation which depends on the instrument and on the resolution of the inversion.

We agree that chi-square fitting has been used to determine the relative weighting of the prior and observational terms, including in Lu et al. (2021), and that the appropriate global factor depends on the inversion setup. Our intention was not to suggest that a global factor cannot be estimated systematically, but rather that a single factor cannot account for spatial variations in observational density. We have revised the text to clarify this distinction and better motivate the density-based weighting approach.

For methane inversions, the choice of γ has relied on L-curve analyses (Hansen, 2000), or approaches that fit a chi-squared distribution to determine the relative weighting of the prior and observational terms (e.g. Lu et al., 2021). Reported values vary substantially depending on model resolution and dataset characteristics (Zhang et al., 2018; Lu et al., 2021; Qu et al., 2021), showing the absence of a universally optimal constant factor. Some of these values have subsequently been adopted in similar inversion configurations (Maasakkers et al., 2019; Zhang et al., 2021). However, a single global factor applies the same adjustment across the observational dataset and cannot account for spatial variations in observation density.

(7) Lines 179–180: Chen et al., 2023 (mentioned above) should really be cited here as the first paper to represent error correlation in super-observations.

Citation included.

(8) Lines 343–345: it would be good to know the spatial and temporal error correlation length scales used for B.

Correlation lengths have been included:

- 500 km spatial horizontal length for all sources.
- 9.5 month temporal length for source "Other".

(9) Line 346: does R also include retrieval and forward model uncertainty? The 3 ppb minimum mentioned here is the kind of number one would get just from the TROPOMI instrument uncertainty (cf. Lorente et al., 2021, paper) but the observational error is much larger, 10–15 ppb, because retrieval and forward model errors dominate. This and other parts of the inversion setup don't bother me too much because the authors are just focusing on the sensitivity to their new scheme, rather than actual inversion results, but this is of some importance in terms of the relative weighting of satellite and surface observations.

General clarification of the paragraph. It now reads as follows:

For the observation error covariance matrix $\mathbf{R}$, the observation uncertainties are specified according to the observation type. For the NOAA surface observations, the uncertainty follows the procedure described in Bergamaschi et al. (2010), using a minimum standard deviation of 3.0 ppb to represent instrumental uncertainty, with additional contributions accounting for temporal and spatial representation errors. These contributions are estimated from model simulations, considering variability within 3-hourly intervals and the impact of local emissions. For the TROPOMI observations, the retrieval uncertainty provided with the data is used, with a minimum standard deviation of 3.0 ppb. No additional spatial or temporal representation errors are included for the satellite observations. Observation errors are assumed to be uncorrelated; thus, $\mathbf{R}$ is constructed as a diagonal matrix containing the resulting observation variances and subsequently inflated using the weighting matrix $\mathbf{\Gamma}$.

(10) Lines 431–433: I don't understand "Consequently, relatively large differences when using the adaptive weighting in underconstrained regions may reflect the spatial distribution of observational constraints and the compensating behavior of the inversion, rather than a corresponding magnitude of error in the prior emissions". The "garbage collector" premise enunciated at the beginning of the paragraph seems weird to me – if adjustment to emissions in a sparsely observed region doesn't significantly improve the cost function then it seems to me that such an adjustment will not be prioritized.

Changed to improve clarity:

> Consequently, differences between inversions using standard and adaptive weighting may be particularly pronounced in these regions, as the weighting scheme changes the relative influence of observations across the domain. Such differences therefore reflect not only potential biases in the prior emissions but also the distribution of observational constraints and the resulting uncertainty in the inferred emissions.

Additional changes

Motivated by the comments from both referees, the discussion of the limitations of the method has been improved in Section 2.3, which now reads as follows:

> The proposed approach has two potential limitations. First, the representativeness effects are accounted for only indirectly, through density-based inflation rather than explicit covariance modeling. Nevertheless, this simplification allows the method to scale efficiently to the large observational datasets typically used in 4DVar inversions. Second, due to the nature of a kernel density estimation, the method does not ensure locally monotonical increasing behavior of the cost function. In practice, for the here used dense TROPOMI data, this behavior has not been observed.

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