**Reduced Cost Construction of Jacobian Matrices for High-Resolution Inversions of Satellite Observations**

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**Abstract**

Global high-resolution observations of atmospheric trace gas concesntrations from satellites can greatly improve our understanding of surface emissions through inverse analyses. For example, the new Tropospheric Monitoring Instrument (TROPOMI) retrieves daily global observations of atmospheric methane concentrations at 7x7 km2 pixel resolution. Variational inverse methods can optimize surface emissions globally at this resolution but do not readily provide error characterization, including information content, for the posterior solution. In fact, the information content of the satellite data may be considerably lower than the data density would suggest because of limited retrieval success rate, instrument noise, and error correlations that propagate through the inversion. This could lead to smoothing errors in variational methods. An analytic inverse solution provides closed-form characterization of the posterior error statistics and information content but requires the construction of the Jacobian matrix relating emissions to atmospheric concentrations. Building the Jacobian matrix is computationally expensive at fine resolution because it involves perturbing each emission element, typically individual grid cells, in the atmospheric transport model. We propose a method to greatly decrease the computational cost of analytic inversions by constructing the Jacobian matrix using only the emission elements with sufficient information content from the observations. Starting from an initial estimate of the Jacobian matrix that assumes simple transport, we iteratively apply perturbations to the leading patterns of information content rather than to the individual model grid cells. The resulting matrix optimizes emissions only in areas spanned by these leading patterns. We demonstrate the method in an analytic Bayesian inversion of GOSAT data over North America in July 2009. We confirm that the estimated Jacobian matrix produces posterior emission estimates and error covariances that are similar to an inversion conducted with the Jacobian matrix for the original model grid. Our method enables computationally efficient, high-resolution analytic inversions of high-density satellite data.

**Section 1: Introduction**

Satellite observations of atmospheric composition provide a resource to improve our understanding of emissions (Streets et al. 2013). However, satellite data are subject to large errors, both from the measurement and from the inverse analyses used to infer emissions from the observations (Brasseur and Jacob 2017). Conducting high-resolution inverse analyses is of considerable interest but may be limited by data quality in ways that are difficult to quantify and that may compromise the results. Here we present two methods to conduct high-resolution inversions of satellite observations that maximize the information content of the observations, minimize computational cost, and provide full error characterization.

Inverse analyses infer emissions by fitting the observed atmospheric concentrations to a chemical transport model (CTM) that simulates atmospheric concentrations as a function of emissions (Brasseur and Jacob 2017). The CTM represents the forward model for the inverse problem. The solution is generally obtained by minimizing a Bayesian cost function regularized by a prior emissions estimate. The optimal (posterior) estimate of emissions corresponds to the minimum of the cost function. This minimum is typically found using a numerical (variational) method, often employing the adjoint of the CTM to compute the cost function gradient (Henze et al. 2007). However, the numerical solution provides no explicit characterization of the solution’s error or information content. While methods of estimating the error exist (Evensen 2009; Bousserez and Henze 2018), these approaches are computationally expensive.

In the frequent case where the observed atmospheric concentrations depend linearly on emissions and the error statistics can be assumed to be normally distributed, the Bayesian optimization problem has an analytic solution including closed-form expressions for the posterior emissions estimate, its error statistics, and its information content (Rodgers 2000). This approach can be extended to non-linear problems and to log-normal error statistics (Maasakkers et al. 2019; Rodgers 2000). The analytic solution requires explicit construction of the Jacobian matrix of the forward model, , which represents the sensitivity of the simulated concentrations to the optimized emission state vector (Brasseur and Jacob 2017). The elements of **y** correspond to individual observations and the elements of **x** correspond to the optimized emission components, often grid cells in a two-dimensional emissions field. The Jacobian can be constructed column-wise by conducting CTM simulations that perturb each of the state vector elements to find the corresponding column (Maasakkers et al. 2019). Even on massively parallel computing clusters, the computational cost of conducting these *n* simulations can limit the size of the state vector **x** and therefore the resolution at which inversions can be conducted (Turner and Jacob 2015). However, once the Jacobian matrix is constructed, inversions can be conducted at essentially no additional computational cost, allowing study of the sensitivity of the solution to changes in the specification of errors, prior assumptions, and the number and type of observations.

An illustrative example is the inversion of satellite observations to infer methane emissions. Methane is an important greenhouse gas but the spatial and temporal distribution of emissions is highly uncertain (Saunois et al. 2019). Satellite observations of atmospheric methane columns can improve emission estimates (Jacob et al. 2016). This was first shown with data from the SCIAMACHY satellite instrument (2003-2012, nadir pixel resolution of 30 x 60 km2) (Bergamaschi et al. 2009, 2013; Houweling et al. 2014; Wecht et al. 2014). More recent inversions used observations from the TANSO-FTS instrument aboard the GOSAT satellite (2009-present) (Monteil et al. 2013; Alexe et al. 2015; Turner et al. 2015; Maasakkers et al. 2019), which measures column methane concentrations in 10-km diameter pixels approximately 250 km apart along- and cross-track (Kuze et al. 2009). The Tropospheric Monitoring Instrument (TROPOMI) aboard the Sentinel-5 precursor, launched in October 2017, now provides daily, global retrievals of atmospheric methane columns at 7 x 7 km2 nadir pixel resolution, increasing coverage by orders of magnitude relative to GOSAT (Veefkind et al. 2012). However, TROPOMI’s methane retrieval has only a ~3% success rate limited by clouds, high aerosol loadings, and variable surface albedo and topography, resulting in heterogeneously distributed observations (Hu et al. 2018). Inversions of TROPOMI data must attempt to capture the high resolution and density of observations where appropriate while recognizing the limitations in information content resulting from data sparsity or errors.

Several methods have been proposed to decrease the computational cost of high-resolution analytic inversions by reducing the dimension or rank of the state vector. Reduced-dimension methods (Bocquet et al. 2011; Turner and Jacob 2015) solve inversions on a multiscale emission grid of dimension *k* < *n* for which the Jacobian matrix can be computed. Bocquet et al. (2011) defined a method to find the optimal multiscale grid from an array of all allowable grids, requiring a large computational investment. Turner and Jacob (2015) used prior emissions information to group together similar grid cells using a Gaussian mixture model, but the criteria used to define similarity were subjective and did not consider the information content of the forward model or observations. Reduced-rank methods (Spantini et al. 2015; Bousserez and Henze 2018) generate a reduced-rank approximation of the inverse solution at the original dimension *n* by solving the inversion in the directions that best explain its information content. Bousserez and Henze (2018) avoided explicit construction of the Jacobian matrix by using randomized methods to estimate these directions. However, this approach is computationally tractable only for inverse systems where a small number of directions explain the information content.

Here we present two methods to construct the Jacobian matrix for a native *n*-dimensional state vector that maximize the information content of the inverse analysis using *k* < *n* forward model simulations. The first method generates a multiscale grid that preserves native resolution where information content is highest and aggregates grid boxes elsewhere. The resulting reduced-dimension Jacobian matrix solves the inversion exactly on the multiscale grid. The second approach constructs the a reduced-rank Jacobian matrix along the dominant patterns of information content in the system, allowing solution of the inversion at native resolution. In both cases, a low-cost initial estimate of the Jacobian matrix is updated using *k* model simulations where *k* is elected by the user and represents a trade-off between computational tractability and information content. We apply both methods to a 1-month inversion of satellite data as demonstration.

**Section 2: Methods**

This section presents both the reduced-dimension and reduced-rank methods of Jacobian matrix construction. Following a review of the standard analytic inverse framework (Section 2.1), we describe optimal reductions in both dimension and rank for an inverse system with a known native-resolution Jacobian matrix (Section 2.2). We then present a two-step update method to approximate the Jacobian matrix using the specified reductions in dimension and rank (Sections 2.3 through 2.5). For the purposes of illustration, we take the state vector to be a gridded field of emissions, although the methods apply to any state vector.

*Section 2.1: Analytic Solution to the Inverse Problem*

The optimal estimate of a state vector **x** given a prior estimate **xA**, observation vector **y**, and normal error statistics given by error covariance matrices **S**Aand **S**O, respectively, is given by the minimization of the Bayesian scalar cost function *J*(**x**):

where **F**(**x)** represents the forward model that simulates the observations **y** (Brasseur and Jacob 2017). The observational error covariance matrix **S**O includes errors from both the measurement and the forward model (collectively the observing system). If the forward model is linear so that **F**(**x**) = **Kx** + **c**, where is the Jacobian matrix calculated via finite difference and **c** is a constant, then an analytic solution to the cost function minimum exists that yields the posterior estimate and its error covariance matrix :

Comparison of and defines the information content of the inverse system, quantified by the averaging kernel matrix , the sensitivity of the posterior emissions estimate to the true state **x**. **A** can be calculated as or as

which expresses the dependence of the averaging kernel matrix on the forward model and both error covariance matrices (Rodgers 2000). The diagonal elements of **A** are commonly referred to as the averaging kernel sensitivities. The sum of the sensitivities, or the trace of **A**, measures the number of pieces of information that can be independently constrained by the inverse system, known as the degrees of freedom for signal or DOFS (Rodgers 2000).

*Section 2.2: Optimal Reductions in Dimension and Rank of Inverse Systems*

We first consider the problem of optimally reducing the dimension and rank of an inverse system with a known Jacobian matrix . Figure 1 illustrates dimension and rank reductions for a hypothetical emission grid over North America. The upper left panel represents the original *n*-dimensional state space, i.e., the native-resolution grid. A linear transformation reduces the dimension of the state space from *n* to *k*. This transformation may reduce dimension discretely, as in the case of grid cell aggregation (upper right panel), or non-discretely, in which case the *k* state vector components are themselves *n*-dimensional vectors (lower right panel). A second linear transformation restores the dimension of the state space from *k* back to the original *n*. The resulting space, depicted in the lower left, is a low-rank approximation of the original state space. The projection transforms the original state space to the low-rank subspace. The inverse problem can be solved in any of these four spaces.

We would like to define matrices and that minimize the information loss associated with reducing the dimension or rank of the state vector. Following Bousserez and Henze (2018), the projection that maximizes the probability of restoring the original full dimension state vector **x** given the reduced dimension state vector is given by where . For a projection of this form, they show that information loss is minimized by maximizing where and **A** are the low-rank and original resolution averaging kernel matrices, respectively (equation (4)). Define

where the columns of **W** are the eigenvectors of and the diagonal elements of are the corresponding eigenvalues of ranked in descending order. Bousserez and Henze (2018) further show that is maximized when where is the matrix of the first *k* columns of **W**, with *k* corresponding to the rank of the projected subspace. The corresponding optimal projection is then

This projection applies a dimension-reducing transformation followed by a dimension-restoring transformation :

The columns of give an eigenvector basis of the averaging kernel matrix while the eigenvalues of **Q** give its eigenvalues. The fraction of information content explained by the first *k* columns of is the sum of the first *k* largest eigenvalues divided by the total DOFS (Bousserez and Henze 2018). We will refer to the rate at which the information content accumulates as the number of eigenvectors increases as the information content spectrum. On the basis of this spectrum, we can select *k* so that most of the information content is explained by the *k* corresponding eigenvectors. Furthermore, the diagonal of

gives the singular values of the pre-whitened Jacobian matrix , representing the signal-to-noise ratio of each eigenvector (Rodgers 2000). The rank *k* can then be chosen so that all eigenvectors have a sufficiently large signal-to-noise ratio. This criterion is stricter than the information content criterion because even eigenvectors with a low signal-to-noise ratio can contribute to the total information content.

*Section 2.3: Approximating the Jacobian Matrix*

Section 2.2. described optimal reductions in dimension and rank of a state vector assuming knowledge of the native-resolution Jacobian matrix **K**. Our goal is to avoid explicit construction of this matrix at native resolution. Here we present a two-step update method to decrease the computational cost of constructing the Jacobian matrix by reducing the dimension and rank of the state vector using the optimal transformations described above. We start from an initial native-resolution estimate and calculate the corresponding averaging kernel matrix . We then consider two methods for updating the Jacobian matrix. In the first method, we construct a multiscale grid that maintains resolution in areas of highest information content (upper right panel of Figure 1) and use the forward model to generate the updated, reduced-dimension Jacobian matrix on the resulting grid. In the second method, we construct on the basis of the *k* dominant eigenvectors by perturbing those patterns in the forward model, generating an approximation of the Jacobian matrix in a reduced-rank state space (lower left panel of Figure 1). In both cases, the updated Jacobian matrix improves the estimate of the averaging kernel matrix and its eigenvectors by incorporating information content from forward model. We use either or to conduct a second update and construct the final Jacobian matrix.

An initial estimate of the native-resolution Jacobian matrix can be generated in our test case by assuming that methane emissions [kg s-1] produce local column concentration enhancements [ppb] dependent on local wind speed and turbulent diffusion. The sensitivity of observation *i* to emissions in grid box *j*, representing the Jacobian matrix element , is given by

where is a factor that decreases with the distance of observation *i* from grid box *j*, and are the molecular weights of dry air and methane, respectively, *g* is gravity, *U* is the local wind speed, *W* is a length scale for the grid cell given by the square root of the grid cell area, and *P* is the surface pressure. The coefficients provide a simple mass-conserving representation of turbulent diffusion and reduce the sparsity of , which is necessary to efficiently generate an updated Jacobian matrix following the two proposed methods. We define for the grid box where the observation is found with the remaining mass distributed over the three concentric rings surrounding that box as 0.3, 0.2, and 0.1.

The initial estimate of the Jacobian matrix can be used to calculate the associated averaging kernel matrix . Because the averaging kernel matrix is a function not only of the Jacobian matrix but of the prior and observational error covariance matrices (equation (4)), this initial estimate will reproduce the patterns of information content determined by the prior errors and observational density despite the crude representation of transport.

*Section 2.4: Constructing the Reduced-Dimension Jacobian Matrix*

In an inverse system with a known native-resolution Jacobian matrix **K**, a reduced-dimension Jacobian matrix can be constructed on a multiscale grid that maintains native resolution where information content is highest and aggregates grid cells elsewhere (upper right panel of Figure 1). An optimal multiscale grid maximizes the total DOFS and the averaging kernel sensitivities of each state vector element, referred to here as the DOFS per cluster. To construct this grid, the state vector is first defined as a single element that encompasses the inversion domain. The native-resolution grid cells with the highest averaging kernel sensitivities are then added to the state vector. For each new element , we calculate the corresponding Jacobian matrix column . In an inversion that optimizes scaling factors, we can easily solve the inversion and calculate the DOFS per cluster. In an inversion optimizing absolute emissions, the sensitivity of the observations to the background cluster must be found for each new state vector. To avoid the added computational cost of this calculation, the inversion can be solved at intervals throughout state vector construction (e.g. after every 50 new state vector elements). In both cases, the DOFS per cluster will increase with the state vector dimension if the observations are able to constrain the new state vector elements. When the DOFS per cluster stops increasing, clusters of two or more native-resolution grid cells are added to the state vector. Clusters are generated by, for example, K-means clustering, which aggregates together spatially proximate grid cells that are likely to yield similar model responses. An algorithm that considers the similarity of emissions, such as the Gaussian mixture model implemented by Turner and Jacob (2015), could also be used. We repeat this process, increasing cluster size, until all native-resolution grid cells are allocated to the multiscale grid and the corresponding reduced-dimension Jacobian matrix is constructed.

Here we use the same approach beginning with our initial estimate in a two-step update process that iteratively improves the multiscale grid. We assume that the fine structure of the averaging kernel sensitivities is given by the prior errors and observational density so that the initial estimate correctly identifies the grid cells with the highest sensitivities. We construct a multiscale grid and the corresponding reduced-dimension Jacobian matrix on the basis of these sensitivities. Constructing the Jacobian matrix introduces information content from the forward model to the inverse system. To identify the state vector elements where the forward model contributes the most information content, we compare the sensitivities given by the updated reduced-dimension averaging kernel matrix to the sensitivities given by the initial estimate regridded onto the multiscale grid. We disaggregate the clusters with the largest difference and update the reduced-dimension Jacobian, generating . The number of clusters disaggregated depends on the magnitude of the differences and on the available computational resources.

The information content associated with both and includes contributions from prior emissions estimates, the observations, and the forward model. As a result, there is rapid convergence and we find that there is no need for further iteration. We therefore take as our Jacobian matrix. The analytic inversion can then be solved exactly on the multiscale grid. In order to interpret the inverse results at the original state vector resolution, additional information must be introduced to allocate the posterior solution to the original grid. The weights could, for example, be given by the prior emissions estimate.

*Section 2.5: Constructing the Reduced-Rank Jacobian Matrix*

In an inverse system with a known native-resolution Jacobian matrix **K**, a reduced-rank approximation of the Jacobian matrix can be constructed by calculating the linear relationship between emissions and observations for the most important patterns of information content rather than for individual or aggregate grid cells. A low-rank Jacobian corresponds to the state space shown in the lower left panel of Figure 1. We showed earlier that the leading patterns of information content are given by the columns of the dimension-restoring transformation (equation (8)). For any selected value of *k*, the *k* leading patterns span a rank *k*, dimension *n* subspace of the original information content space. A Jacobian matrix can be constructed within this space by calculating the model response to perturbations of these patterns. The response of a forward model **F** to the *j*th eigenvector , given by the *j*th column of , is

where is any scalar sufficiently large to ensure numerical stability. The model responses form the columns of the matrix, which is the Jacobian for an inverse system with a reduced-dimension state space spanned by the first *k* eigenvectors of the information content, illustrated by the lower right panel of Figure 1. This reduced-dimension Jacobian must be transformed to the original state dimension to enable physical interpretation of inverse results. Bousserez and Henze (2018) show that the reduced-dimension Jacobian matrix is given by and the reduced-rank Jacobian matrix by Thus, the reduced-rank Jacobian can be calculated from the reduced-dimension Jacobian by . The resulting Jacobian has dimension and rank .

In an inverse system without a known Jacobian matrix, the reduced-rank Jacobian matrix approximation can be constructed in a two-step update that iteratively improves the patterns of information content used as perturbations. We use the initial estimate of the Jacobian matrix to calculate the corresponding averaging kernel matrix and the matrix of its eigenvectors . When calculating , we select the eigenvectors that have a signal-to-noise ratio greater than or equal to about 1 (equation (9)). We use a strict signal-to-noise threshold to account for the errors in the initial estimate of the information content. We calculate the model response to each of the eigenvectors using equation (9) and transform the resulting reduced-dimension Jacobian to the full-dimension state space with .

The reduced-rank Jacobian matrix approximation introduces information from the forward model to the inverse system, improving the characterization of the eigenvectors of information content relative to the native-resolution system. We calculate the associated averaging kernel matrix and the matrix of its eigenvectors . Because is a reduced-rank approximation, its spectrum of information content is discontinuous at . To select the rank of the second update and calculate , we therefore use the spectrum of information content associated with the initial, full-rank estimate . While is not informed by the forward model, we expect that it captures with some accuracy the spectrum of information content because much of its structure is determined by the prior error covariance matrix and observational density (Section 2.1). We use the eigenvectors that span most of the information content from the initial estimate to construct an updated reduced-rank Jacobian matrix approximation as above. The resulting Jacobian matrix is a rank approximation that accurately quantifies the forward model where the inverse system has high information content as and loses accuracy in areas with lower information content where the observations are least able to constrain emissions.

**Section 3: Results and Discussion**

We demonstrate both the reduced-dimension and reduced-rank Jacobian matrix construction approaches in an analytic Bayesian inversion of atmospheric methane columns observed by the GOSAT satellite over North America in July 2009. Although TROPOMI now provides higher density observations, using GOSAT allows us to follow the framework developed by Maasakkers (2019) to construct a “native-resolution” inverse system at 1º x 1.25º grid cell resolution (*n* = 2098, upper left panel of Figure 1) against which our reduced-dimension and reduced-rank methods can be compared. To demonstrate the applicability of the methods to inversions of TROPOMI data, we artificially increase the information content of the GOSAT data by introducing a regularization factor to the cost function that increases the weight of the observational terms relative to the prior terms:

The regularization factor functionally decreases the observational error covariance, increasing the DOFS. We set . In the native-resolution inversion, this increases the DOFS from 40 to 216. The significant increase in DOFS also generates large negative scaling factors in the posterior solution; the unphysical solution does not affect our demonstration.

We use the nested North American GEOS-Chem CTM version 12.4.0 as forward model to simulate atmospheric methane column concentrations at 0.5º x 0.625º resolution for July 2009. We aggregate native resolution grid boxes to generate a state vector composed of 2098 1º x 1.25º grid boxes. The model is driven with MERRA-2 meteorological fields (Bosilovich et al., 2016) from the NASA Global Modeling and Assimilation Office (GMAO). We use boundary conditions and initial conditions from a global posterior GEOS-Chem 4º x 5º simulation from Maasakkers et al. (2019). Relative prior emissions, relative prior error covariances, observations, and observational error covariances are also as described by Maasakkers et al. (2019). In particular, we use the GOSAT data from the University of Leicester version 7 CO2 proxy retrieval over land (Parker et al. 2011, 2015) for July 2009. Unlike Maasakkers et al. (2019), we use observations north of 60ºN; any large errors in these data do not matter for the sake of our demonstration. After constructing the native-resolution Jacobian matrix, we use it to as the forward model in lieu of additional GEOS-Chem simulations.

Figure 2 (upper left panel) shows the averaging kernel sensitivities of the native-resolution averaging kernel matrix **A**. As discussed in Section 2 and illustrated in Figure 2, the sensitivity patterns are largely driven by the prior error standard deviation (lower left panel) and the observation density (lower right panel) due to the large variability in these terms. The variability in the prior error standard deviation is driven by the spatial variability of the prior methane emissions because the errors are relative to those emissions. The variability in observation density is driven by variability in sampling and retrieval success, which depends in part on surface reflectivity and the presence of a clear sky.

Figure 2 (upper right panel) also shows the initial estimate of averaging kernel sensitivities derived from the initial estimate of the Jacobian matrix following the approach described in Section 2.3. While no forward model simulations were conducted to construct this initial estimate, the patterns of information content as given by the sensitivities closely reproduce those given by the native-resolution averaging kernel matrix **A** because of the strong dependence on the prior error standard deviation and observation density.

We first construct a reduced-dimension Jacobian on a multiscale grid. Figure 3 shows the evolution of the DOFS per cluster as a function of the number of native resolution grid cells added to the state vector as increasingly coarse state vector elements, aggregated by a K-means clustering algorithm and color coded by cluster size, are added to the multiscale grid. We begin with a state vector with one domain-encompassing element. To account for the functional decrease in the observational error covariance resulting from the increase in the number of observations constraining each state vector element, we scale down the regularization factor introduced in equation (10) by the ratio of the new state vector dimension to the native state vector dimension. As result of this scaling, the initial DOFS per cluster is less than one. We add to this single element state vector the native resolution grid cells with the highest estimated averaging kernel sensitivities as given by . We add 50 cells at a time to reproduce the construction of the multiscale grid in a parallel computing environment. The DOFS per cluster decreases initially because the high-resolution grid cells have lower DOFS. After adding 150 native-resolution grid cells (151 model simulations, including the single state vector element simulation), we find that the DOFS per cluster consistently decreases and that the maximum DOFS per cluster occurred at 80 native-resolution grid cells (black shading). We then add to our state vector of 80 native-resolution grid cells clusters of first ~2 (purple shading), then ~4 (maroon), ~8 (dark orange), ~16 (light orange), and ~32 (yellow) native-resolution grid cells, repeating the same procedure as before: we add clusters in batches of about 50 (and then 25) until the DOFS per cluster decreases or stabilizes, at which point we increase the cluster size. The resulting multiscale grid is summarized in the table at the bottom of Figure 3; the reduced-dimension Jacobian matrix constrains 359 clusters and required 470 model simulations to construct.

We then update the multiscale grid and the reduced-dimension Jacobian matrix to reflect the information added by the forward model. We identify the clusters where the forward model contributed the most information by regridding the sensitivities given by to the multiscale grid and calculating the change in the sensitivities. We find that the sensitivity of 165 clusters increased, 162 of which were clusters of 2 or more native-resolution grid cells. We disaggregate 16 clusters with a sensitivity increase greater than 0.4, adding 64 native-resolution grid cells and forward model simulations. Disaggregating additional clusters would increase the number of forward model simulations beyond the computational limit of 600 model runs for this demonstration. The updated multiscale grid increases the resolution of the inverse solution, increases the total DOFS from 79 to 89, and maintains the DOFS per cell at 0.21.

Figure 4 shows the final multiscale grid. The final multiscale grid has dimension 423 and the corresponding reduced-dimension Jacobian matrix required 534 forward model simulations. The final grid has 199 native-resolution grid cells and clusters ranging from size 1 to size 58. The variability in cluster size relative to the sizes stated above results from the K-means clustering algorithm.

The grid maintains native resolution where information content is highest (upper left panel of Figure 2), notably over the Gulf Coast and Southeast coast, California’s Central Valley, and South-central Canada. Grid cells are aggregated elsewhere, notably over the American West and western, northern, and eastern Canada, where there is low observation density (lower right panel of Figure 2).

We solve the analytic inversion on this grid and compare the results to the native-resolution solution. Figure 5 shows the averaging kernel sensitivities (top) and posterior emission scaling factors (bottom) for the reduced-dimension solution (center column) compared to the native-resolution solution (left column). Both solutions are exact on the grids used. The reduced-dimension solution generates fewer DOFS (89) than the native-resolution solution (216) but twice as many DOFS per cell (0.21 compared to 0.10), reflecting the consolidation of information content. This is reflected in the plotted sensitivities: the reduced-dimension solution has more uniform sensitivities relative to the native-resolution solution. The reduced-dimension posterior scaling factors exhibit less variability than the native-resolution values. However, some of the variability in the native-resolution solution is attributable to the large regularization factor, which causes “checker-boarding” where the posterior solution fits observational noise. The reduced-dimension scaling factors successfully capture the native-resolution regional patterns.

We next construct a reduced-rank Jacobian matrix. We calculate the dominant eigenvectors of the initial averaging kernel matrix estimate, requiring that the signal-to-noise ratio of all eigenvectors be greater than 2, corresponding to 44% of the DOFS and *k* = 92. We perturb these eigenvectors in the forward model and construct the reduced-rank Jacobian matrix as described in Section 2.5 using the native resolution Jacobian matrix as the forward model. We recalculate averaging kernel matrix and its dominant eigenvectors. The eigenvalue spectrum given by the updated information content has a discontinuity at *n* = 113 as expected for a rank 113 system. We use the initial eigenvalue spectrum to determine *k* for the second update, requiring that the improved eigenvectors capture 98% of the information content, corresponding to *k* = 437. The resulting Jacobian matrix has rank ~437 and required 530 forward model simulations including the prior run, a 75% reduction from the 2099 simulations required for the native-resolution solution.

We solve the inversion (equations (2) – (4)) using and compare the information content to the native-resolution solution. The top row of figure 4 shows the distribution of the reduced-rank averaging kernel sensitivities (right) compared to the native resolution solution (left). Because was constructed on the basis of the dominant patterns of information content, it solves for the posterior scaling factors in the areas of highest information content and defaults to the prior value (a scaling factor of 1) elsewhere. Visual inspection suggests that the reduced-rank averaging kernel sensitivities accurately capture these patterns of information content. The lower right panel of figure 5 confirms this conclusion. We show the reduced-rank averaging kernel sensitivities greater than 0.01 plotted against the corresponding native-resolution values. The reduced-rank sensitivities correlate strongly (R = 0.91) with the native-resolution values. The underestimate of the reduced-rank sensitivities reflects the loss of information content in the reduced-rank solution; the reduced-rank DOFS (153) and DOFS per grid cell (0.07) are lower than native-resolution values (216 and 0.10, respectively). If we consider only the optimized grid cells (averaging kernel sensitivities greater than 0.01), we find 152 DOFS across 679 grid cells, or 0.22 DOFS per grid cell. The reduced-rank solution generates only ~70% of the native-resolution DOFS despite constructing the reduced-rank Jacobian matrix on the basis of eigenvectors that capture 98% of the information content; the discrepancy results from errors in the characterization of the tailing eigenvectors.

We also compare the reduced-rank posterior scaling factors to the native-resolution solution. The bottom row of figure 4 shows the distribution of the reduced-rank (right) and native-resolution (left) posterior scaling factors. The reduced-rank solution captures the native-resolution solution where the averaging kernel sensitivities are highest. The upper right panel of figure 5 supports this conclusion: the filtered reduced-rank posterior scaling factors correlate strongly with the native-resolution values (R = 0.87). The correlation is lower than that exhibited by the Jacobian matrix elements (upper left, R = 0.97), posterior variances (lower left, R = 0.98), and averaging kernel sensitivities due to the propagation of errors (equation (2)). While the reduced-rank inversion underestimates the averaging kernel sensitivities and overestimates the posterior variances, reflecting the loss of information content, the error in the posterior scaling factors appears random.

We conduct a series of sensitivity tests on the number of model runs used in both the first and second update. Figure 6 summarizes these results. We show the DOFS plotted against the number of model runs conducted in the first and second iteration. As expected, the DOFS increase with the total number of model runs. We find that the DOFS have a stronger dependence on the number of model runs conducted in the second iteration, consistent with the improved characterization of the information content after the first iteration and confirming that it is preferable to increase the number of model runs in the second iteration if additional computational resources are available.

**Section 4: Conclusions**

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