*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**. However, the *n* + 1 forward model simulations needed to construct **K** may be prohibitively expensive. Here we present a two-step approach to construct a reduced-dimension or reduced-rank Jacobian matrix at much lower computational cost. We start from a low-cost, native-resolution estimate (see below) and calculate the corresponding averaging kernel matrix . In the reduced-dimension method, we use to construct a multiscale grid that maintains resolution in the areas of highest information content (top right panel of Figure 1). We generate the updated, reduced-dimension Jacobian matrix on the resulting grid using the forward model. In the reduced-rank method, we construct on the basis of the *k* dominant eigenvectors of by perturbing those patterns in the forward model, generating an approximation of the Jacobian matrix in a reduced-rank state space (bottom left panel of Figure 1). In both methods, 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.

In our demonstration case, we generate a native-resolution Jacobian matrix at no cost by assuming that a perturbation of methane emissions [kg m-2 s-1] produce local dry column mixing ratio enhancements [mol mol-1] as determined by a simple column mass balance dependent on local wind speed and parameterized turbulent diffusion. We construct row-wise by assuming that observation *i* responds to emissions in grid cell *j* as

and therefore

where is a dimensionless coefficient providing a crude representation of turbulent diffusion, and are the molecular weights of dry air and methane, respectively, *L* is a ventilation length scale taken as the square root of the grid cell area, *g* is gravitational acceleration, *U* is the local wind speed taken here as 5 km h-1, and *p* is the surface pressure. We assume 0.4 for observations in grid cell *j* and distribute the remaining mass over the three concentric rings surrounding that cell with = 0.3/8, 0.2/16, and 0.1/24 from the inner to outer ring. This representation of turbulent diffusion reduces the sparsity of and expands the footprint of the dominant patterns of information content; the exact parameterization (e.g. the number of rings used or the values of ) is unimportant.

The reduced-dimension and reduced-rank methods rely on characterizing the dominant patterns of information content of the observing system using the initial estimate of the averaging kernel matrix . can provide a good approximation of **A** even if the initial estimate of the Jacobian matrix is crude because the averaging kernel matrix depends strongly on the specified prior and observational error covariance matrices and (equation (4)) and because, by assuming that observed concentrations are most sensitive to local emissions, generates the highest information content where the observations are densest. This structure can then be refined by a two-step update.