A low-rank approach to the solution of weak constraint variational data assimilation problems.

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Introduction

Data assimilation is a way of combining observations with a numerical model, to create a better estimate of the true state.

We propose an approach for implementing the weak four-dimensional variational data assimilation method with a low-rank solution in order to achieve a reduction in storage space. We have

- A state $x_k \in \mathbb{R}^n$ at time t_k, with $x_{k+1} = \mathcal{M}_k(x_k) + \eta_k$.
- A background estimate x^b of the truth x_0^* with $x_0^* = x^b + e_0$
- Observations $y_k = \mathcal{H}_k(x_k^*) + \epsilon_k \in \mathbb{R}^{p_k}$.

$\mathcal{M}_k$ and $\mathcal{H}_k$ are (potentially non-linear) model and observation operators. We assume the errors η_k, e_0, ϵ_k are Gaussian with zero mean and covariances Q_k, B and R_k respectively. Weak four dimensional variational data assimilation (Weak 4D-Var) minimises the cost function

$$J(x) = \|x_0 - x_0^b\|^2_{B^{-1}} + \sum_{k=0}^{N} \|y_k - \mathcal{H}_k(x_k)\|^2_{R_k^{-1}} + \sum_{k=1}^{N} \|x_k - \mathcal{M}_k(x_{k-1})\|^2_{Q_k^{-1}},$$

which is a weighted least squares to the background, observations, and the model trajectory.

Incremental 4D-Var

Incremental 4D-Var is a form of Gauss-Newton iteration. The 4D-Var cost function is approximated by a quadratic function of an increment

$$\delta x^{(\ell)} = \left[(\delta x_0^{(\ell)})^T, (\delta x_1^{(\ell)})^T, \ldots, (\delta x_N^{(\ell)})^T\right]^T,$$

with $\delta x^{(\ell)} = x^{(\ell+1)} - x^{(\ell)}$, and iterate (ℓ).

At the minimum we have

$$\nabla \tilde{J}(\delta x) = L^T D^{-1}(L\delta x - b) + \mathrm{H}^T \mathrm{R}^{-1}(\mathrm{H}\delta x - d) = 0.$$

Taking $M_k \in \mathbb{R}^{n\times n}$ and $H_k \in \mathbb{R}^{n\times p_k}$, as the linearisations of $\mathcal{M}_k$ and $\mathcal{H}_k$ about $x^{(\ell)}$, we let

$$L = \mathrm{tridiag}([-M_1, \cdots, -M_N], I, 0),$$
$$D = \mathrm{diag}(B, Q_1, \cdots, Q_N),$$
$$\mathrm{R} = \mathrm{diag}(R_0, \cdots, R_N), \quad \mathrm{H} = \mathrm{diag}(H_0, \cdots, H_N),$$
$$b = \left[b_0^T, c_1^T, \cdots, c_N^T\right]^T, \quad d = \left[d_0^T, d_1^T, \cdots, d_N^T\right]^T,$$

where

$$b_0^{(\ell)} = x_0^b - x_0^{(\ell)}, \quad c_k^{(\ell)} = \mathcal{M}_k(x_{k-1}^{(\ell)}) - x_k^{(\ell)},$$
$$d_k^{(\ell)} = y_k - \mathcal{H}_k(x_k^{(\ell)}).$$

Saddle point formulation

Let $\lambda = D^{-1}(b - L\delta x)$ and $\mu = \mathrm{R}^{-1}(d - \mathrm{H}\delta x)$, at the minimum we have

$$\nabla \tilde{J} = L^T\lambda + \mathrm{H}^T\mu = 0. \quad (1)$$

Additionally, we have

$$D\lambda + L\delta x = b, \quad (2)$$
$$\mathrm{R}\mu + \mathrm{H}\delta x = d, \quad (3)$$

and (1), (2) and (3) can be combined to give:

$$\begin{bmatrix} D & 0 & L \\ 0 & \mathrm{R} & \mathrm{H} \\ L^T & \mathrm{H}^T & 0 \end{bmatrix} \begin{bmatrix} \lambda \\ \mu \\ \delta x \end{bmatrix} = \begin{bmatrix} b \\ d \\ 0 \end{bmatrix}, \quad (4)$$

which is solved for δx.

Kronecker formulation

We may rewrite the saddle point matrix as

$$\begin{bmatrix} E_1 \otimes B + E_2 \otimes Q & 0 & I \otimes I_n + C \otimes M \\ 0 & I \otimes R & I \otimes H \\ I \otimes I_n + C^T \otimes M^T & I \otimes H^T & 0 \end{bmatrix},$$

where we make the additional assumptions that $Q_k = Q$, $R_k = R$, $H_k = H$, $M_k = M$ and the number of observations $p_k = p$ for each k. Here $C = \mathrm{tridiag}(-1, 0, 0)$,

$$E_1 = \begin{bmatrix} 1 & & \\ & 0 & \\ & & \ddots & \\ & & & 0 \end{bmatrix}, \quad \text{and } E_2 = \begin{bmatrix} 0 & & \\ & 1 & \\ & & \ddots & \\ & & & 1 \end{bmatrix}.$$

The matrices $C, E_1, E_2, I \in \mathbb{R}^{N+1\times N+1}$, whilst $B, Q, M, I_n \in \mathbb{R}^{n\times n}$, $H \in \mathbb{R}^{p\times n}$, and $R \in \mathbb{R}^{p\times p}$.

Simultaneous Matrix Equations

Using the identity $(\mathcal{B}^T \otimes \mathcal{A})\mathrm{vec}(\mathcal{C}) = \mathrm{vec}(\mathcal{ACB})$, we obtain the simultaneous matrix equations:

$$B\Lambda E_1 + Q\Lambda E_2 + X + MXC^T = \mathbb{b},$$
$$RU + HX = \mathrm{d},$$
$$\Lambda + M^T\Lambda C + H^T U = 0.$$

where $\lambda, \delta x, b, \mu$ and d are vectorised forms of the matrices $\Lambda, X, \mathbb{b} \in \mathbb{R}^{n\times N+1}$ and $U, \mathrm{d} \in \mathbb{R}^{p\times N+1}$ respectively. Let us now suppose the matrices Λ, U, X have low-rank representations,

$$\Lambda = W_\Lambda V_\Lambda^T, \quad U = W_U V_U^T, \quad X = W_X V_X^T.$$

Low-Rank GMRES

We use GMRES despite the symmetric matrix to experiment with constraint preconditioners. To implement a low-rank version of GMRES, we need:

Vector addition

Vectors in GMRES become vectorised matrices, so $X_{k1} = [Y_{k1}, \ Z_{k1}]$, $X_{k2} = [Y_{k2}, \ Z_{k2}]$ for $k = 1, 2, 3$ gives addition, and $x = y + z$ is

$$\mathrm{vec}\left(\begin{bmatrix} X_{11}X_{12}^T \\ X_{21}X_{22}^T \\ X_{31}X_{32}^T \end{bmatrix}\right) = \mathrm{vec}\left(\begin{bmatrix} Y_{11}Y_{12}^T + Z_{11}Z_{12}^T \\ Y_{21}Y_{22}^T + Z_{21}Z_{22}^T \\ Y_{31}Y_{32}^T + Z_{31}Z_{32}^T \end{bmatrix}\right).$$

Matrix vector products come from the simultaneous matrix equations, giving $\hat{X}_{ij}$ after multiplication by the saddle point matrix

$$\hat{X}_{11} = [BX_{11}, QX_{11}, X_{31}, MX_{31}],$$
$$\hat{X}_{12} = [E_1X_{12}, E_2X_{12}, X_{32}, CX_{32}],$$
$$\hat{X}_{21} = [RX_{21}, HX_{31}],$$
$$\hat{X}_{22} = [X_{22}, X_{32}],$$
$$\hat{X}_{31} = [X_{11}, M^TX_{11}, H^TX_{21}],$$
$$\hat{X}_{32} = [X_{12}, C^TX_{12}, X_{22}].$$

Inner products

$$\langle w, v^{(i)}\rangle = \mathrm{trace}\left(W_{11}^T V_{11}^{(i)} (V_{12}^{(i)})^T W_{12}\right) + \mathrm{trace}\left(W_{21}^T V_{21}^{(i)} (V_{22}^{(i)})^T W_{22}\right) + \mathrm{trace}\left(W_{31}^T V_{31}^{(i)} (V_{32}^{(i)})^T W_{32}\right).$$

Truncating after concatenation steps, we obtain a low-rank implementation of GMRES.

Numerical experiments with 1D advection-diffusion

We consider the 1D advection-diffusion system, with a discretisation of $n = 100$, and $N + 1 = 200$ assimilation steps. We take partial, noisy observations in all 200 timesteps with $p = 20$, and observations at every fifth component. The covariances are $B_{i,j} = 0.1\exp(\frac{-|i-j|}{50})$, $Q = 10^{-4}I_{100}$, $R = 0.01I_{20}$, leading to a saddle point system of size 44,000.

We compare the root mean squared error (RMSE) of our low-rank implementation, the full-rank case (solving the saddle point system using backslash), and the background estimate with no assimilation.

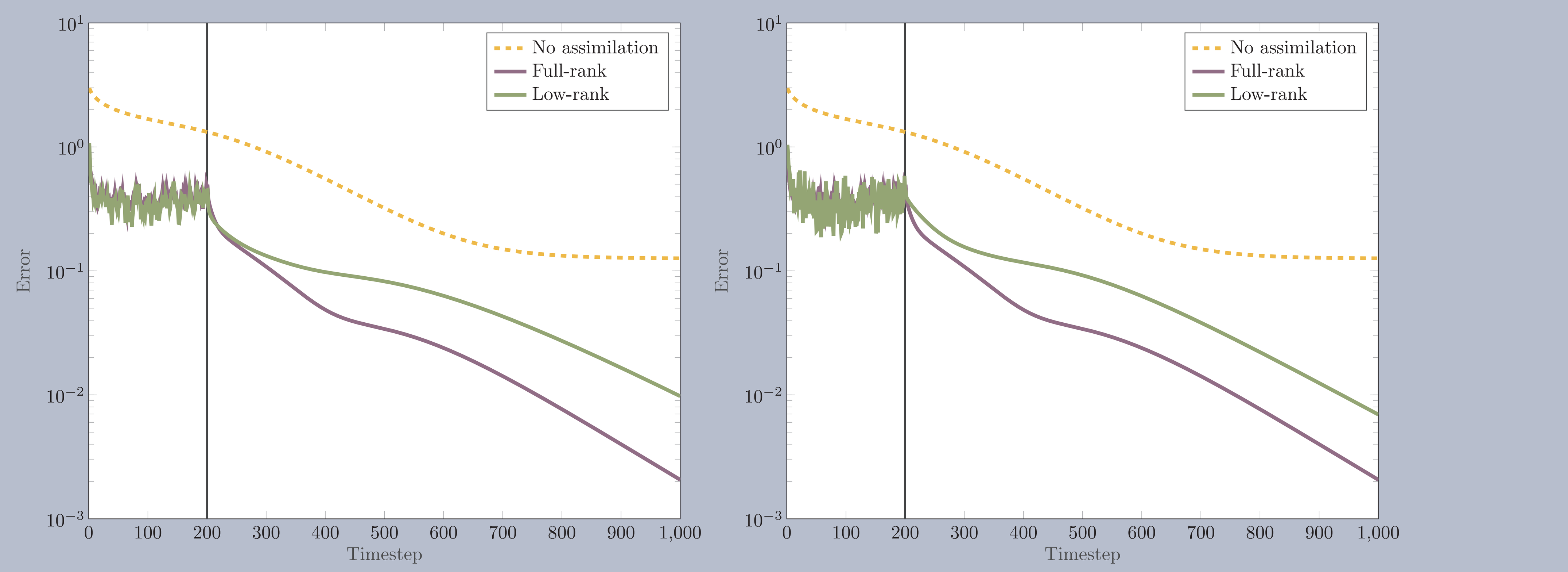

Figure 1: RMSE for 1D A-D problem with partial, noisy observations, $(r = 20)$ on left, $(r = 5)$ on right.

We see the low-rank approach achieves similar results to the full-rank case, and importantly significantly better than performing no assimilation on our initial guess.

These low-rank solutions result in storage reductions of 70 and 92.5% respectively, requiring 6,000 or 1,500 entries as opposed to 20,000.

Conclusions

Weak constraint 4D-Var is a very large optimisation problem, however we have shown that under certain assumptions, low-rank solutions exist. Experimentally this appears to be the case under relaxed assumptions also. We have also found that preconditioning may not be necessary, with the low-rank approach acting like a regularisation. For more information and references, please see:

[1] M. A. Freitag and D. L. H. Green. A low-rank approach to the solution of weak constraint variational data assimilation problems. ArXiv e-prints, 1702.07278